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Handbook of Thermodynamic Diagrams



Volume 2

Organic
Compounds
C₅ to C₇

Carl L. Yaws

LIBRARY OF PHYSICO-CHEMICAL PROPERTY DATA

Handbook of Thermodynamic Diagrams



Volume 2

Organic
Compounds
C₅ to C₇

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LIBRARY OF PHYSICO-CHEMICAL PROPERTY DATA

Handbook of Thermodynamic Diagrams



Volume 2

Organic
Compounds
C₅ to C₇

Carl L. Yaws



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Handbook of Thermodynamic Diagrams, Volume 2

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CONTENTS

Preface	vii
Thermodynamic Graphs for Organic Compounds C_5 to C_7	1
References	368
Appendix A: Equations for Thermodynamic Properties	370
Appendix B: Peng-Robinson Equation of State for Thermodynamic Properties	371
Appendix C: Examples for Thermodynamic Diagrams	373
Appendix D: Critical Constants and Acentric Factor for C_5 to C_7 Compounds	375
Appendix E: Gas Heat Capacity for C_5 to C_7 Compounds	380
Compound List by Formula	386
Compound List by Name	393
Computer Program for Thermodynamic Properties	400

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DISCLAIMER

This handbook presents a variety of thermodynamic and physical property data. It is incumbent upon the user to exercise judgment in the use of the data. The author and publisher do not provide any guarantee, express or implied, with regard to the general or specific applicability of the data, the range of errors that may be associated with any of the data, or the appropriateness of using any of the data in any subsequent calculation, design, or decision process. The author and publisher accept no responsibility for damages, if any, suffered by any reader or user of this handbook as a result of decisions made or actions taken on information contained herein.

PREFACE

Thermodynamic property data are important in many engineering applications in the chemical processing and petroleum refining industries. The objective of this book is to provide the engineer with such data. The data are presented in thermodynamic diagrams (graphs) covering a wide range of pressures and temperatures to enable the engineer to quickly determine values at points of interest. The contents of the book are arranged in the following order: graphs, references, and appendixes.

The graphs are arranged by carbon number and chemical formula to provide ease of use. English units are used for the property values. For those involved in SI and metric usage, each graph displays a conversion factor to provide the SI and metric units.

The graphs provide wide coverage for volume and enthalpy as a function of temperature and pressure, including the following:

- two-phase region for saturated liquid and vapor
- superheated gas region for gases above saturation temperature
- subcooled liquid region for liquids below saturation temperature
- supercritical region for temperatures and pressures above critical point

The graphs for enthalpy also contain lines of constant entropy to permit engineering usage for 2nd law problems such as adiabatic expansion and compression of fluids.

The coverage encompasses a wide range of organic compounds including hydrocarbons, such as alkanes, olefins, acetylenes, and cycloalkanes; oxygenates, such as alcohols, aldehydes, ketones, acids, ethers, glycols, and anhydrides; halogenates, such as chlorinated, brominated, fluorinated, and iodinated compounds; nitrogenates, such as nitriles, amines, cyanates, and amides; sulfur compounds, such as mercaptans, sulfides, and sulfates; silicon compounds, such as silanes and chlorosilanes; and many other chemical types.

The range of coverage for pressure is from 10 to 10,000 psia. Very limited experimental data are available at pressures above 1,000 to 2,000 psia. Thus, values at the higher pressures should be considered rough approximations. Values at lower pressures are more accurate.

The graphs are based on the Peng-Robinson equation of state (1) as improved by Stryjek and Vera (2, 3). The equations for thermodynamic properties using the Peng-Robinson equation of state are given in the appendix for volume, compressibility factor, fugacity coefficient, residual enthalpy, and residual entropy. Critical constants and ideal gas heat capacities for use in the equations are from the data compilations of DIPPR (8) and Yaws (28, 29, 30).

The literature has been carefully searched in construction of the graphs. References for sources used in preparing the work are given in the section following the graphs near the end of the book.

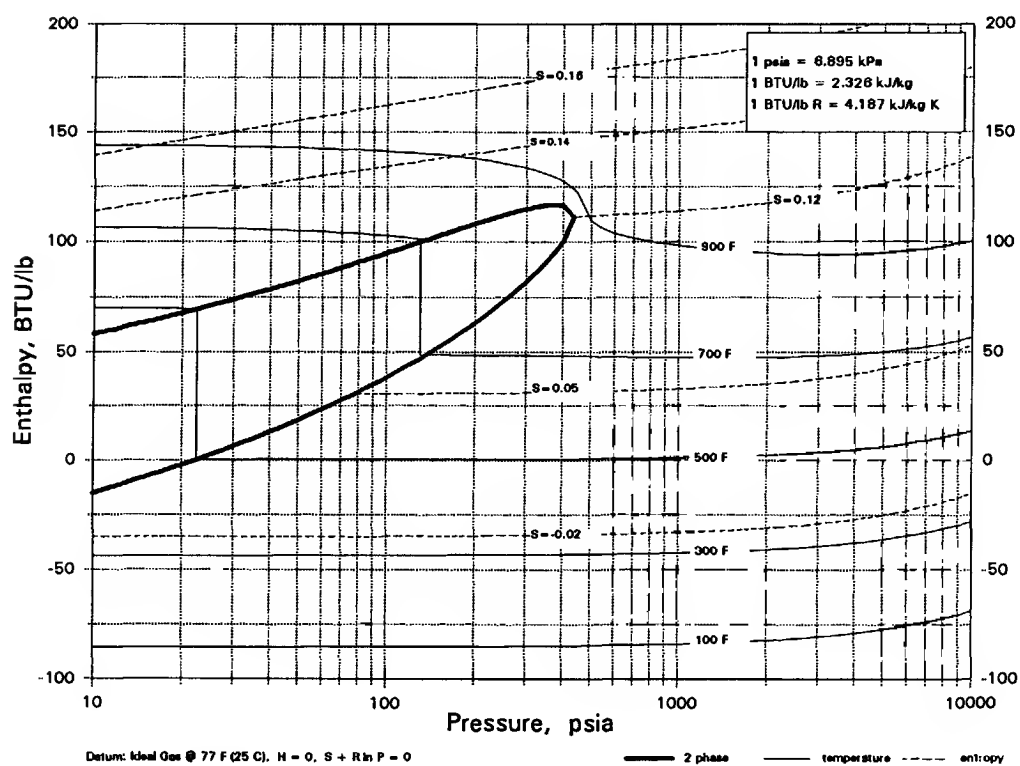
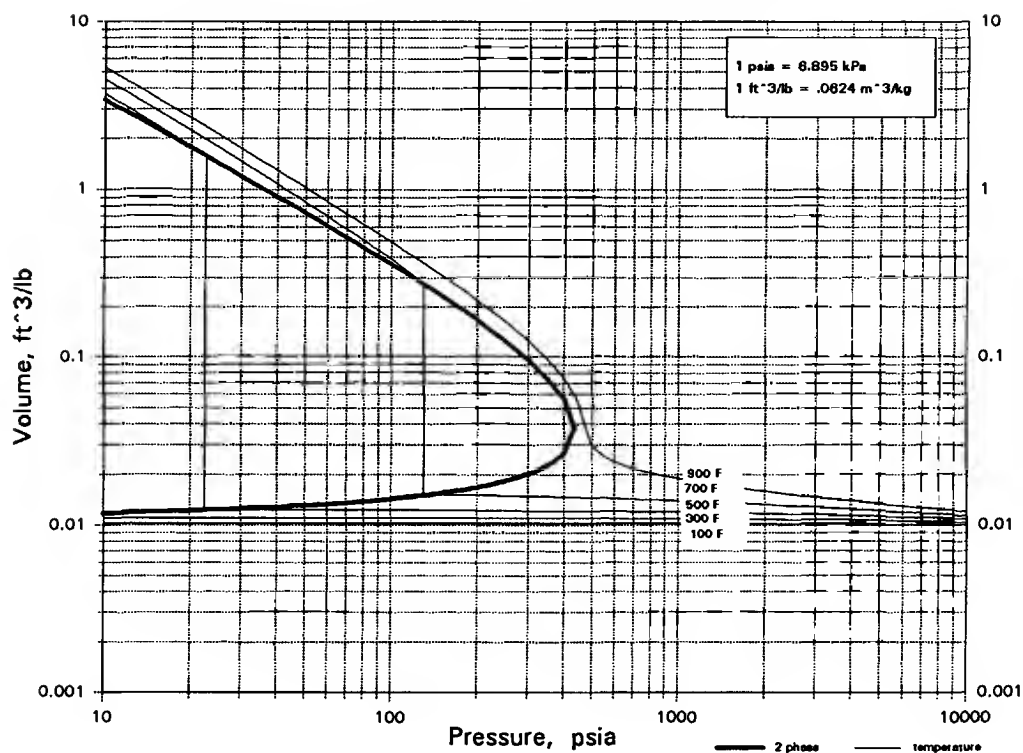
For the graphs, some of the compounds may undergo thermal decomposition (reaction) at the higher temperatures. For such cases of thermal decomposition, the graphs are useful for ascertaining property values of the pure compound which is contained in the reaction mixture. Chemistry handbooks and DIPPR (8) notes may be used for specifics regarding thermal decomposition.

A list of compounds is given near the end of the book to aid the user in quickly locating compounds of interest from knowledge of the chemical formula or name.

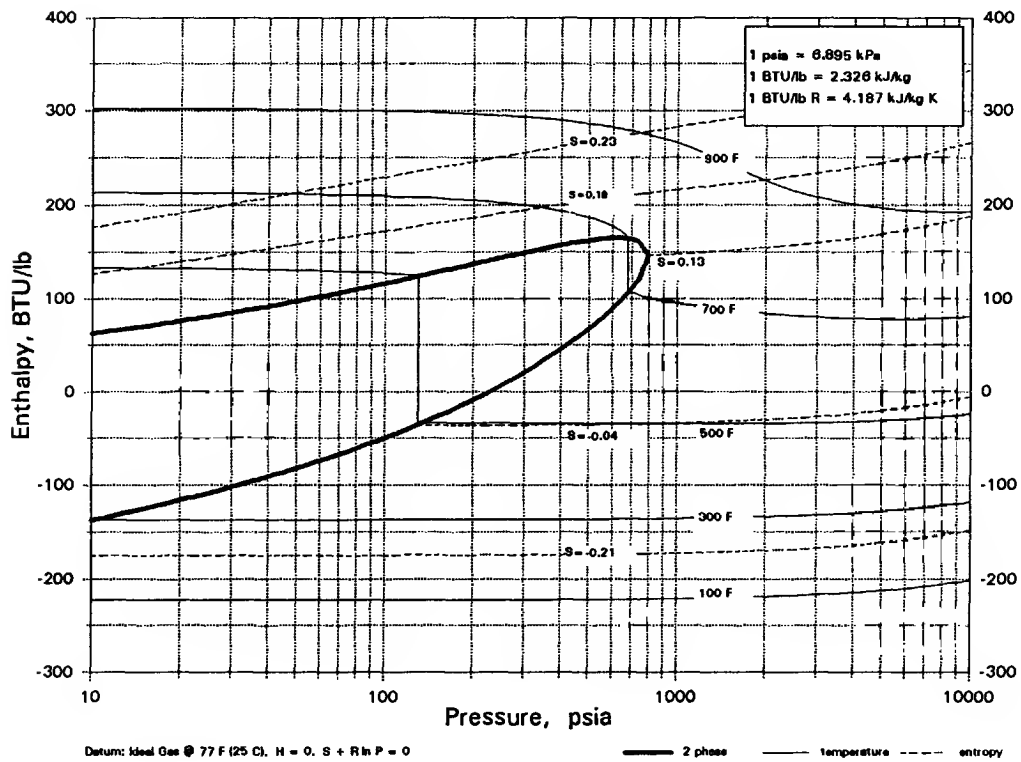
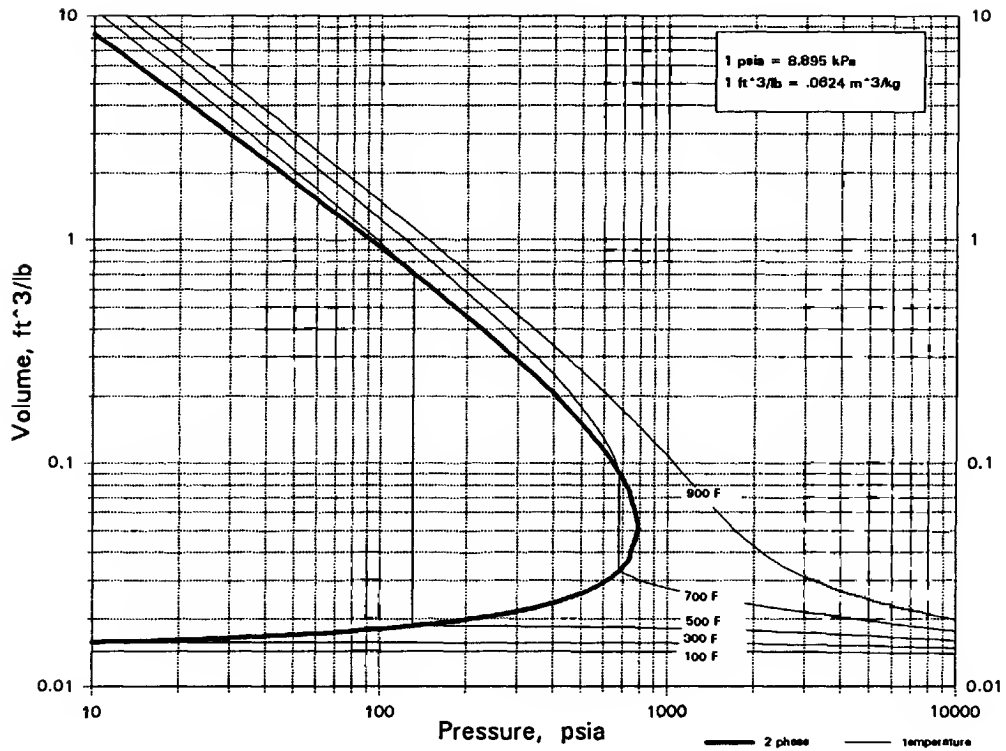
An executable computer program, complete with data files, is available for calculation of thermodynamic properties. For information on the program, contact Carl L. Yaws, Ph.D., P. O. Box 10053, Beaumont, Texas 77710, phone/fax (409) 880-8787.

C5Cl6

HEXACHLOROCYCLOPENTADIENE

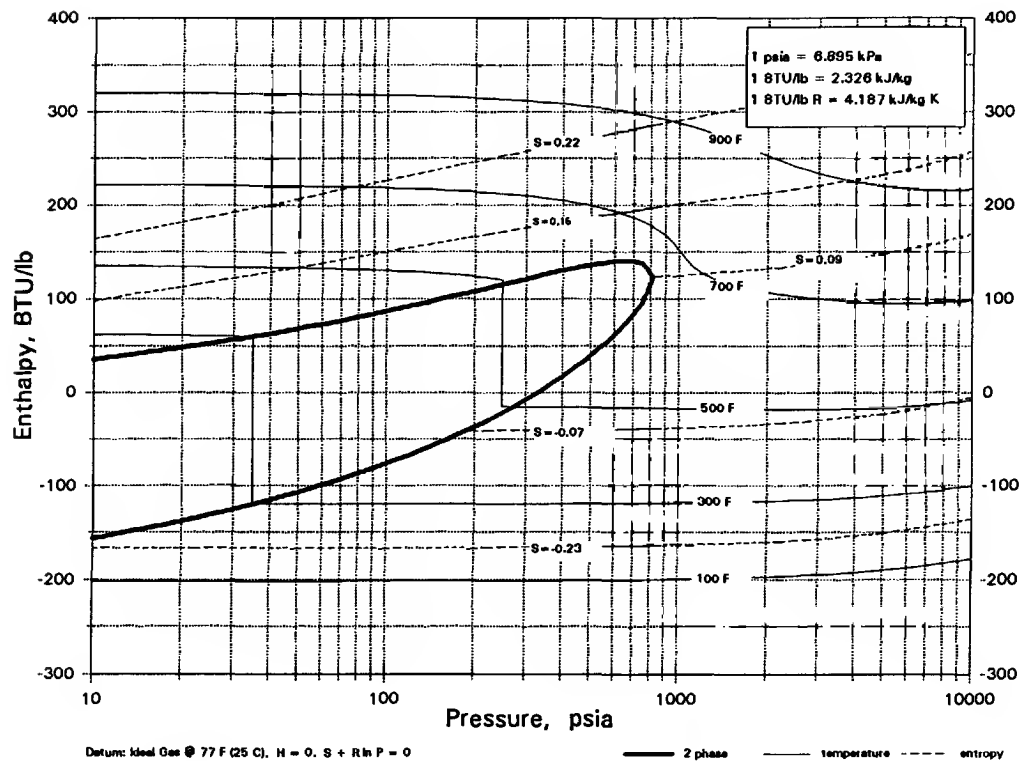
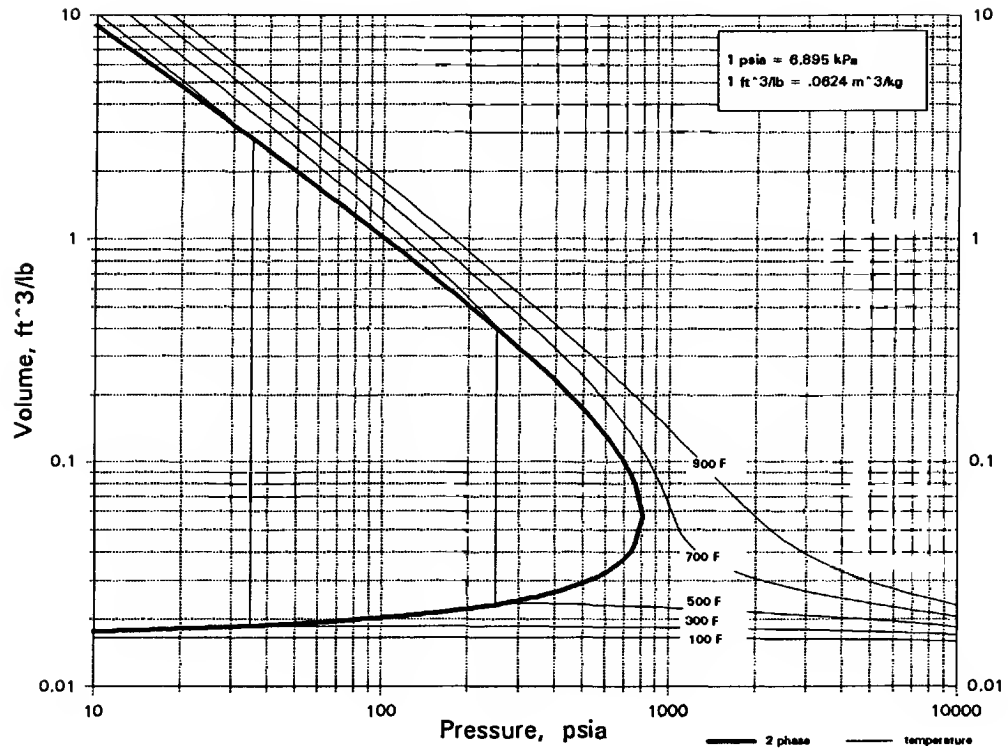


C5H4O2
FURFURAL



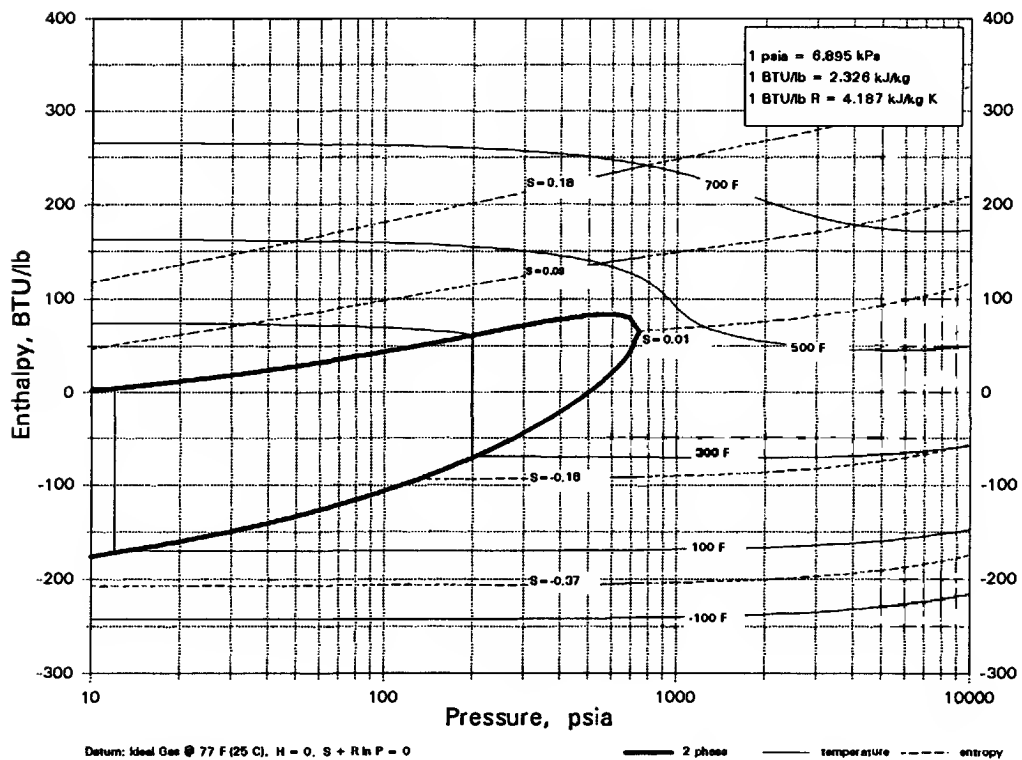
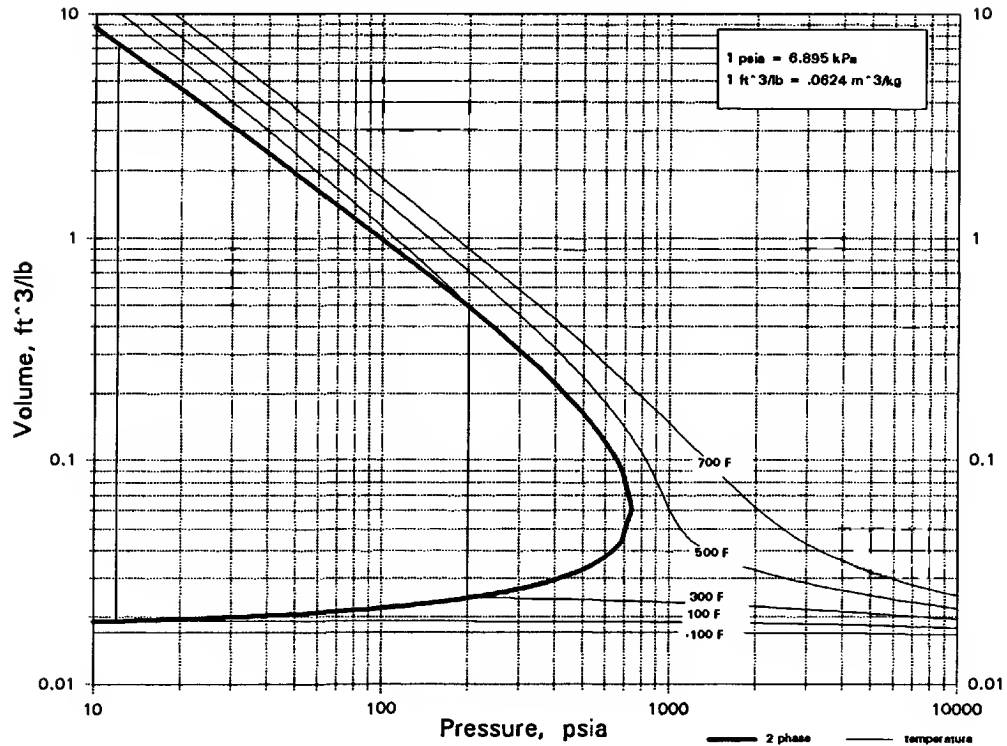
C5H5N

PYRIDINE



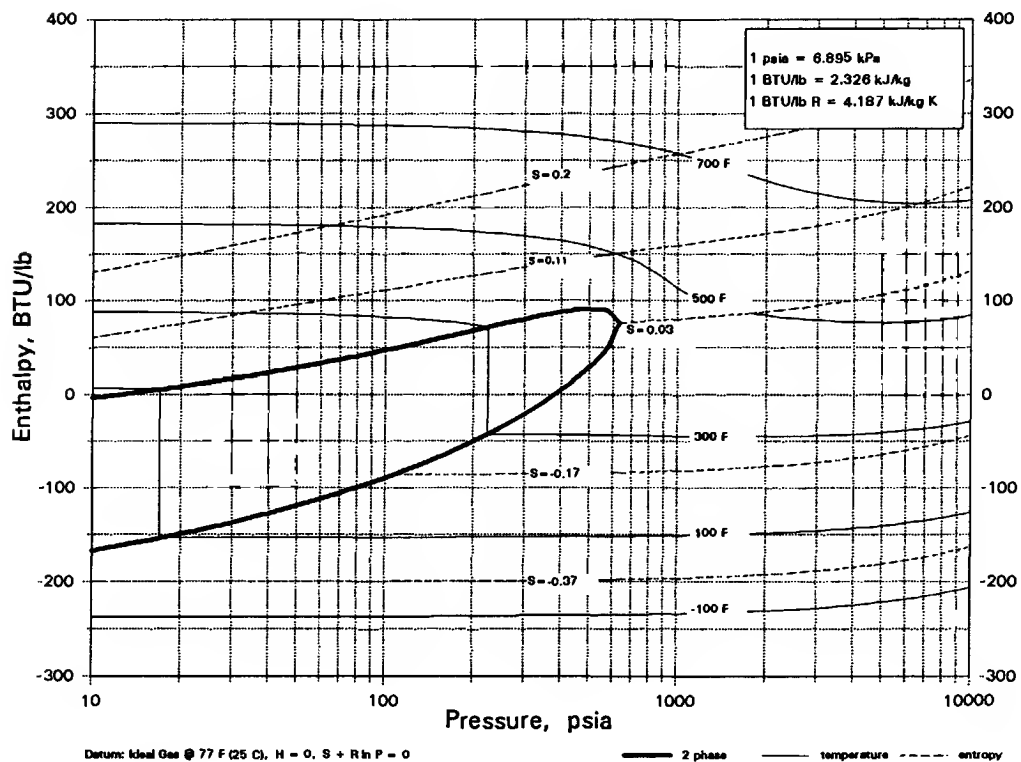
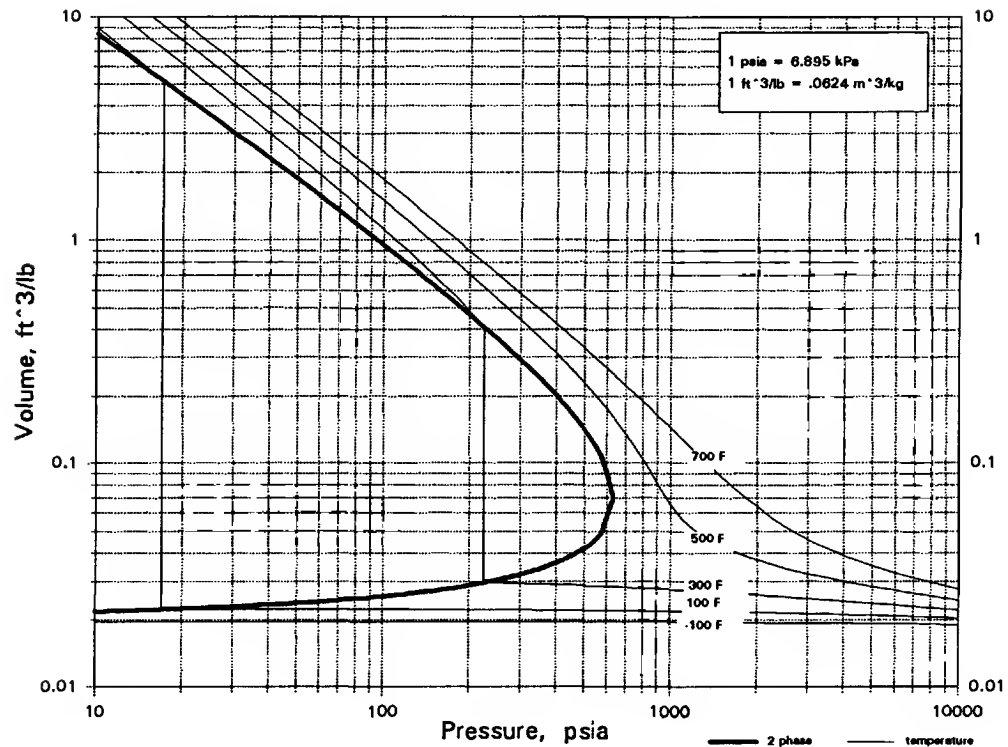
C5H6

CYCLOPENTADIENE



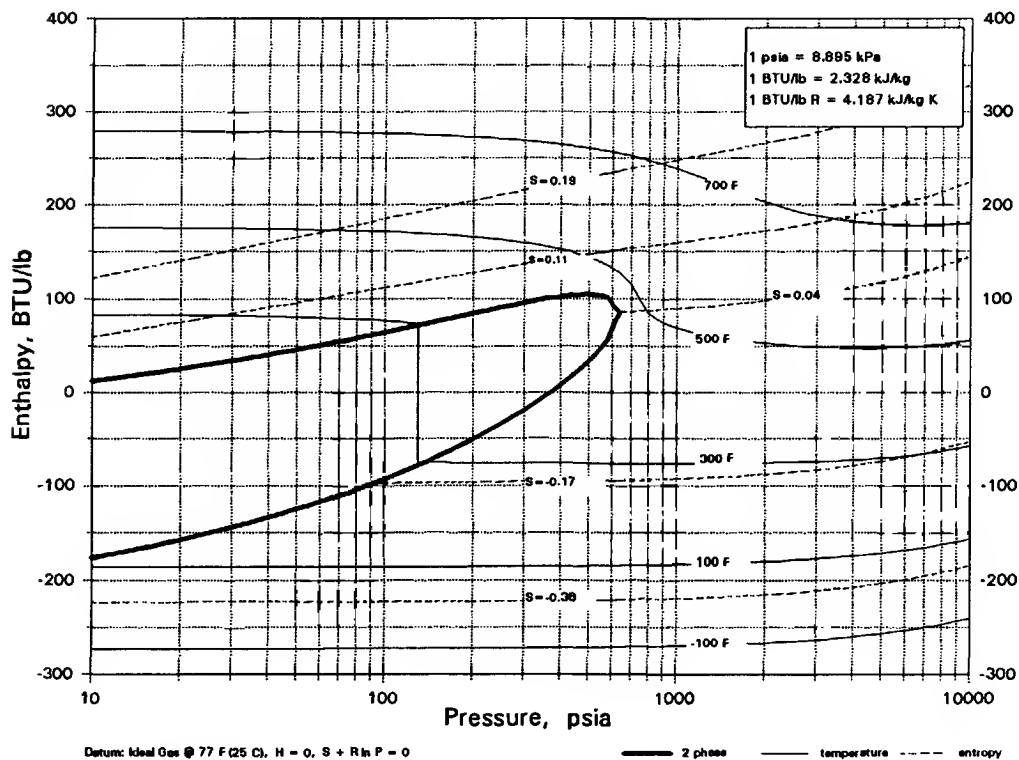
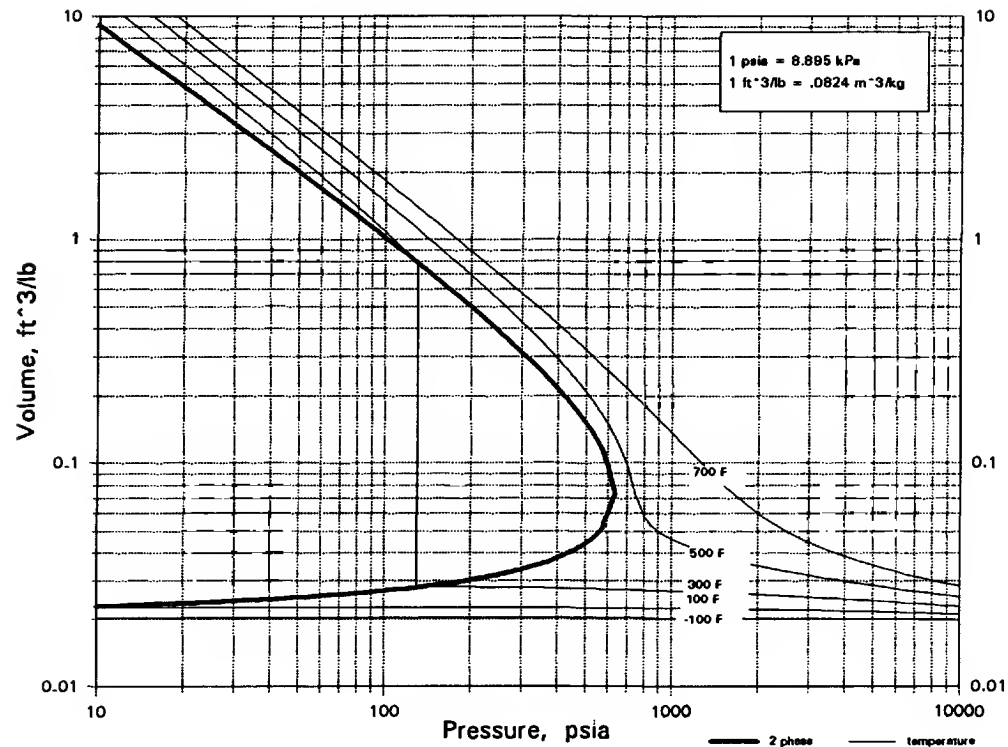
C5H6

2-METHYL-1-BUTENE-3-YNE



C5H6

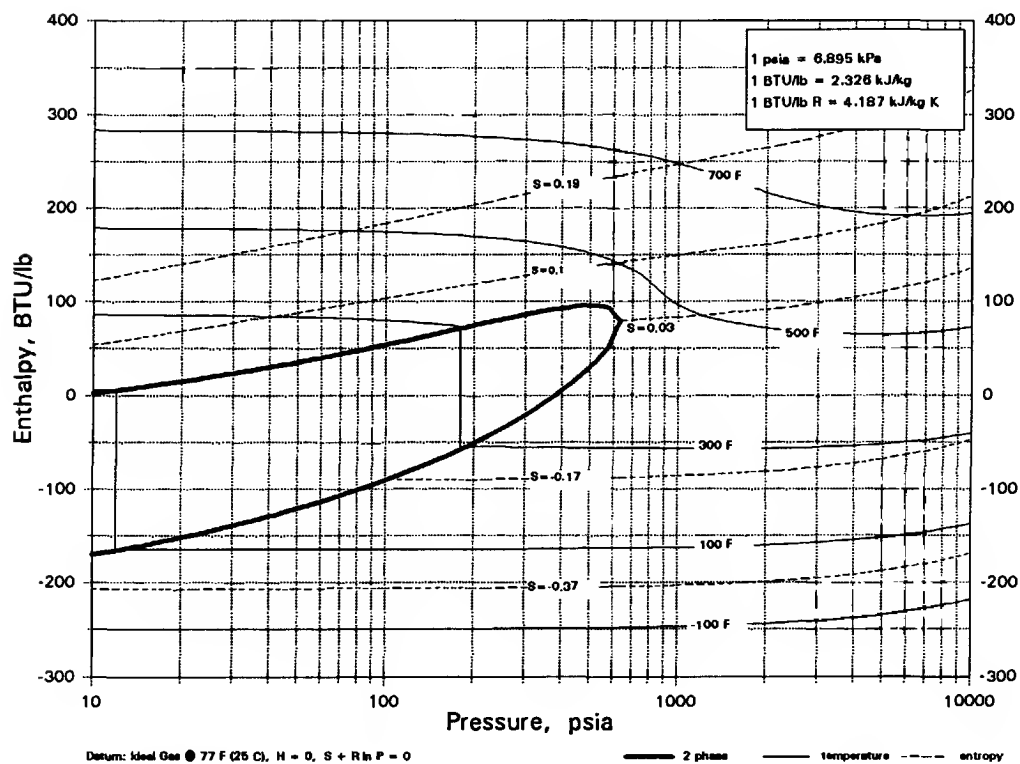
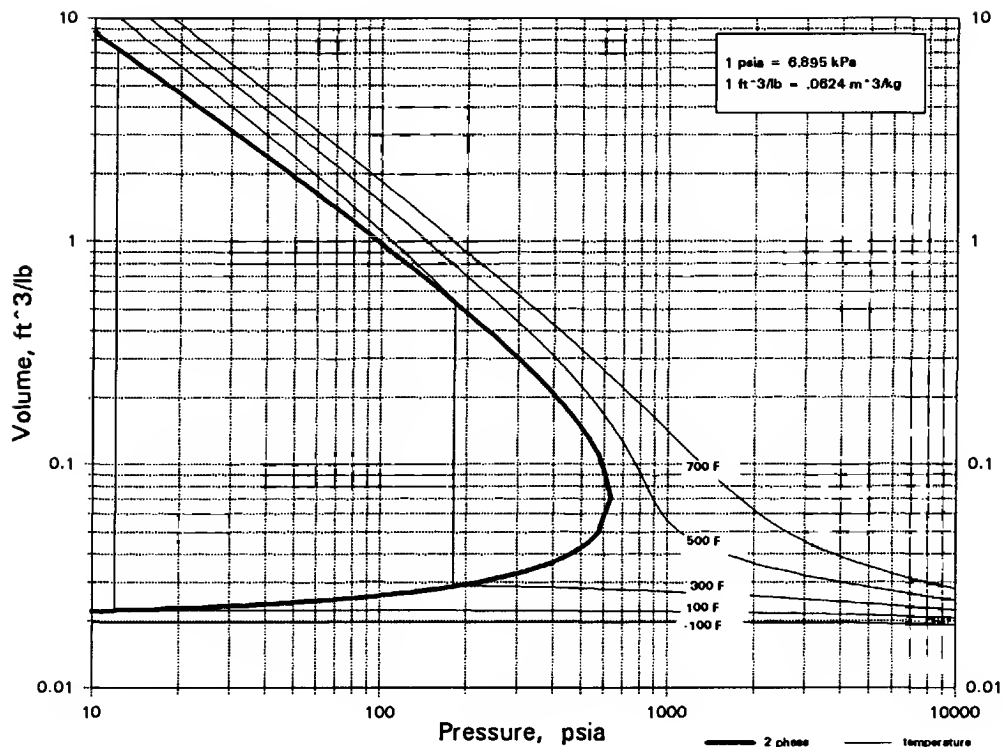
1-PENTENE-3-YNE



Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

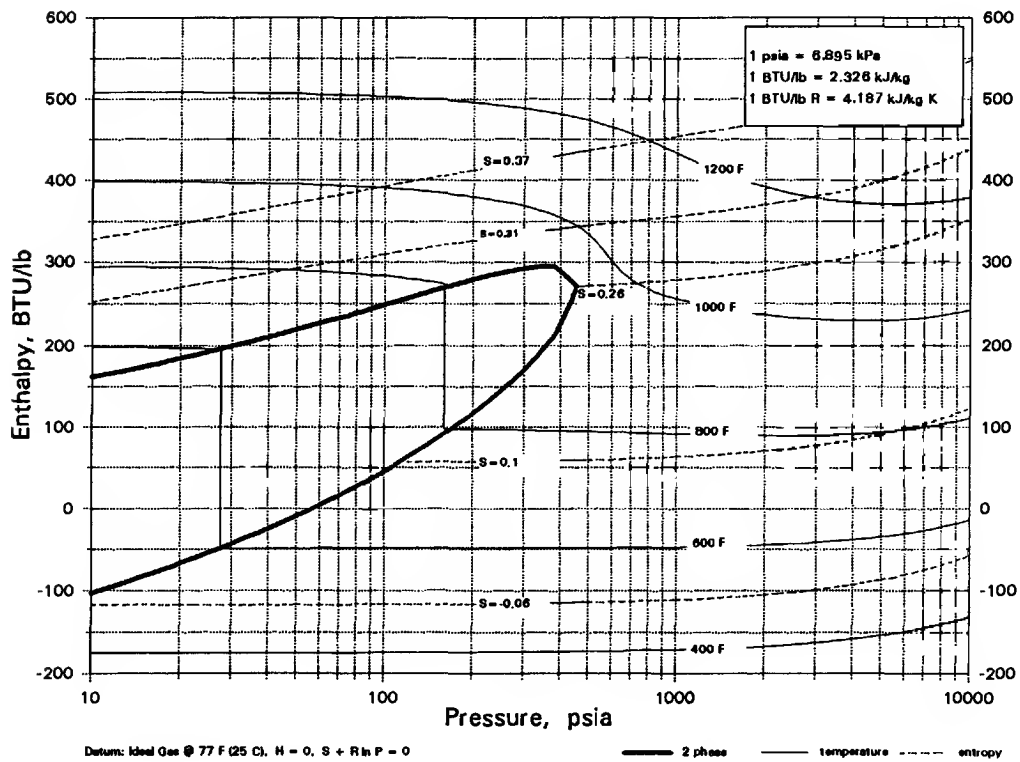
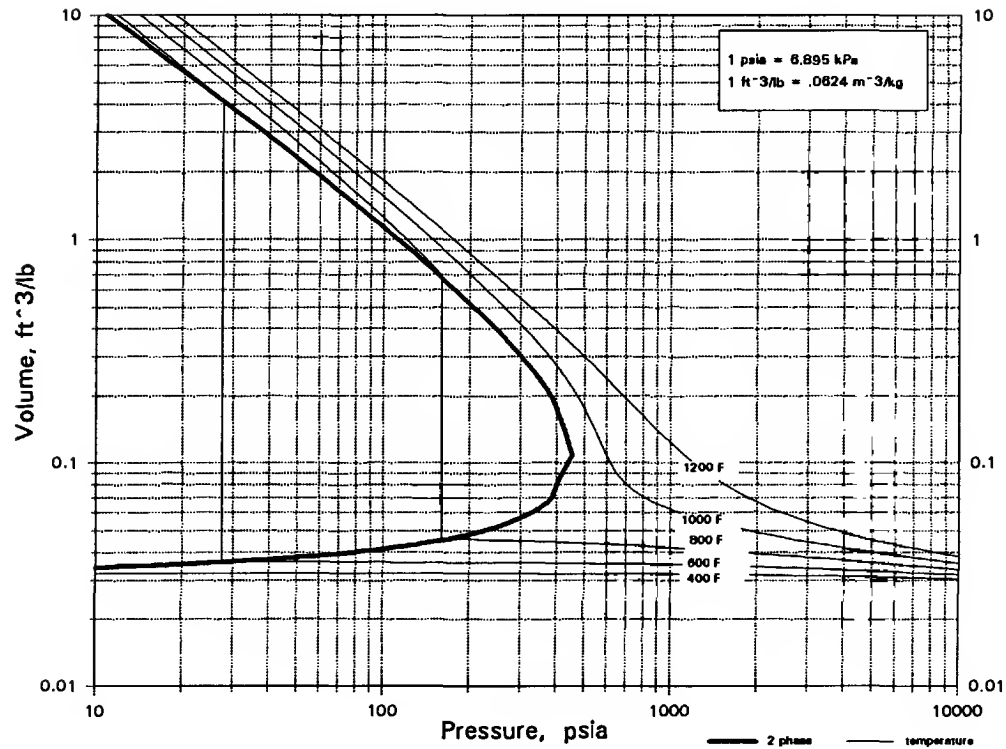
C5H6

1-PENTENE-4-YNE



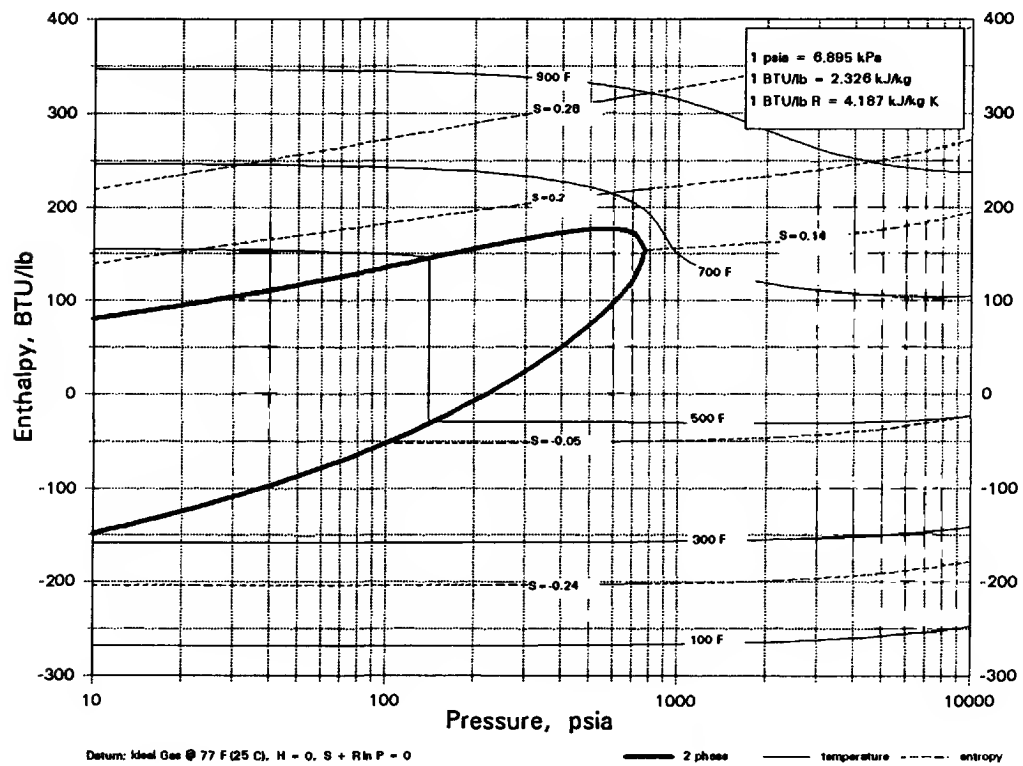
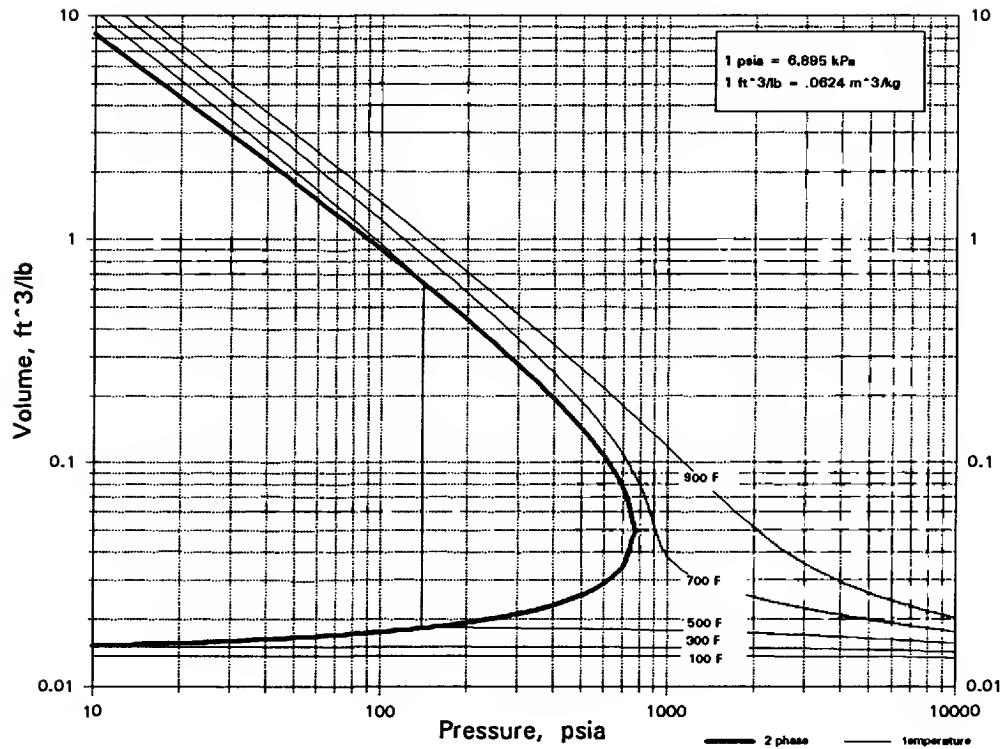
C5H6N2

GLUTARONITRILE

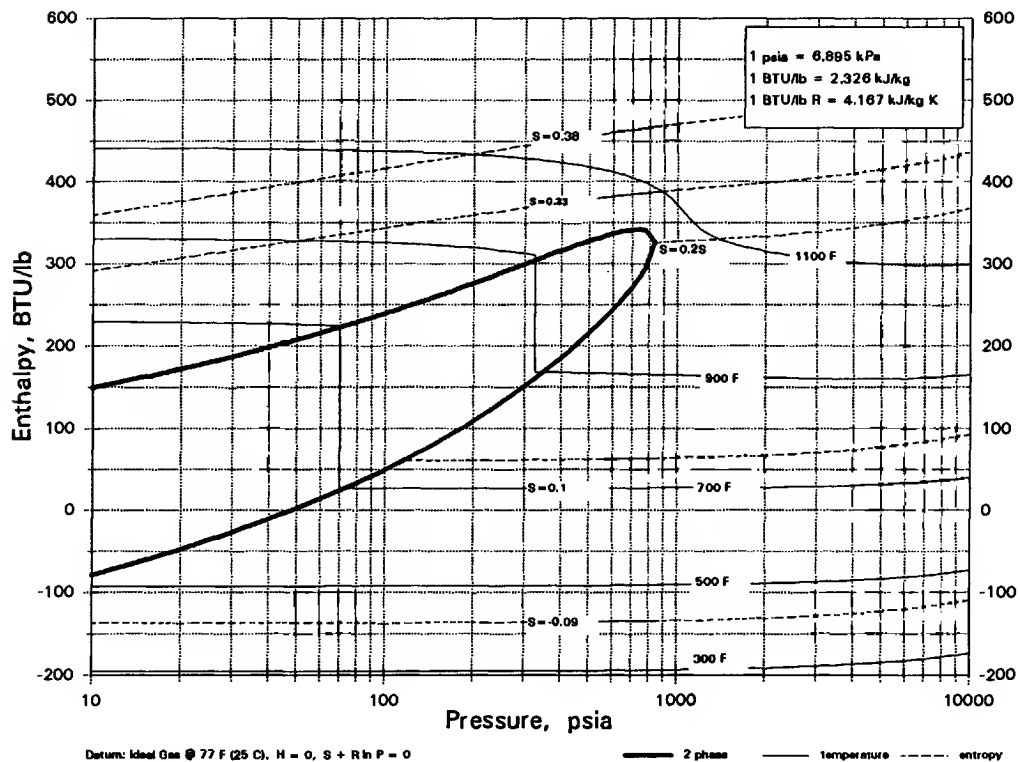
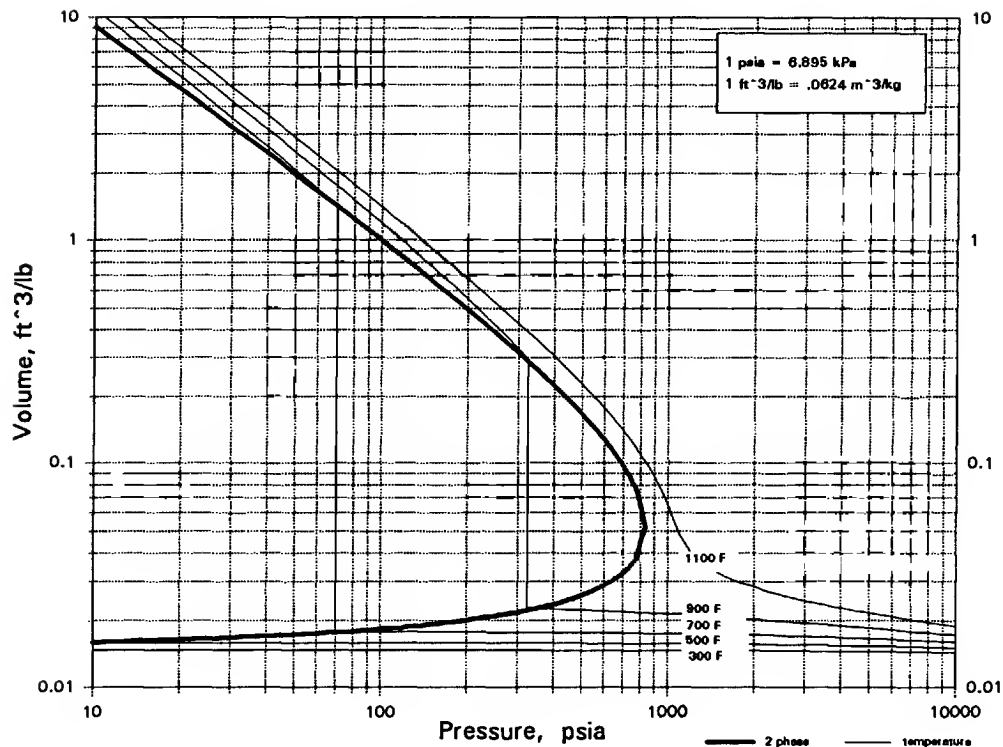


C5H6O2

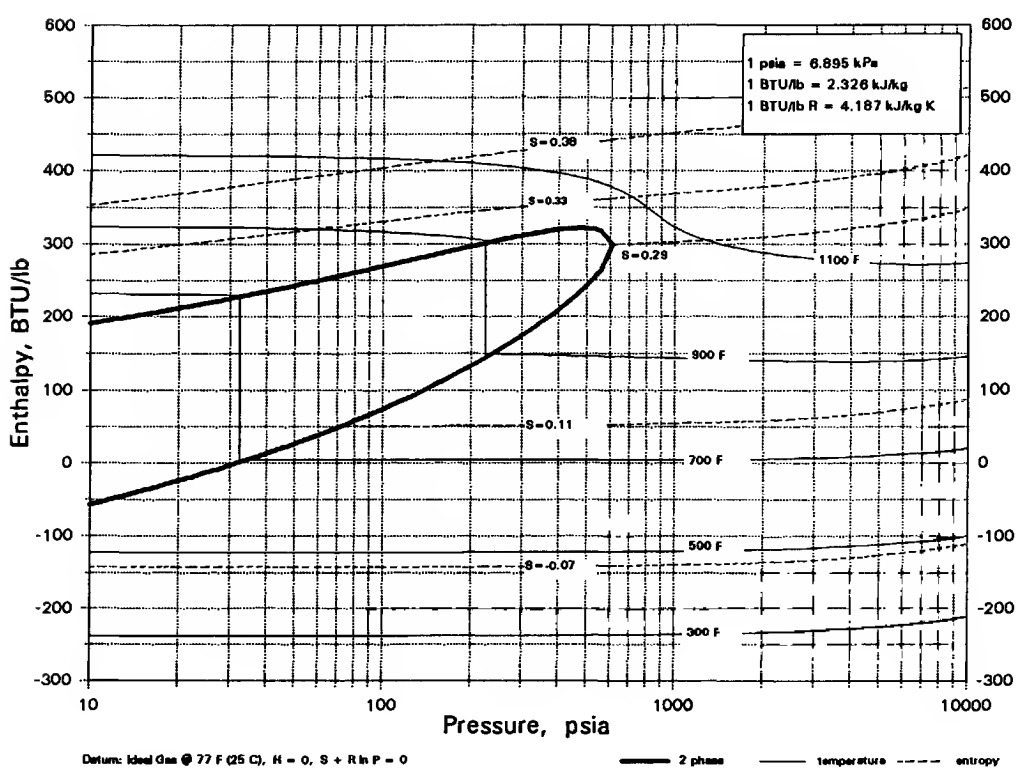
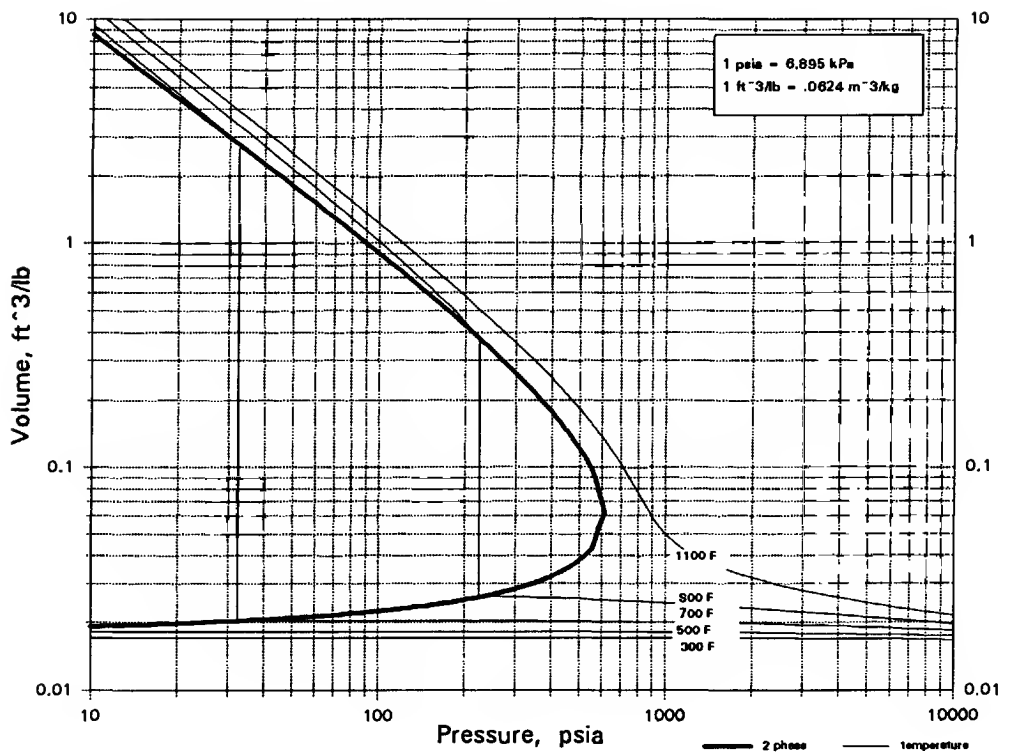
FURFURYL ALCOHOL



C5H6O3
GLUTARIC ANHYDRIDE

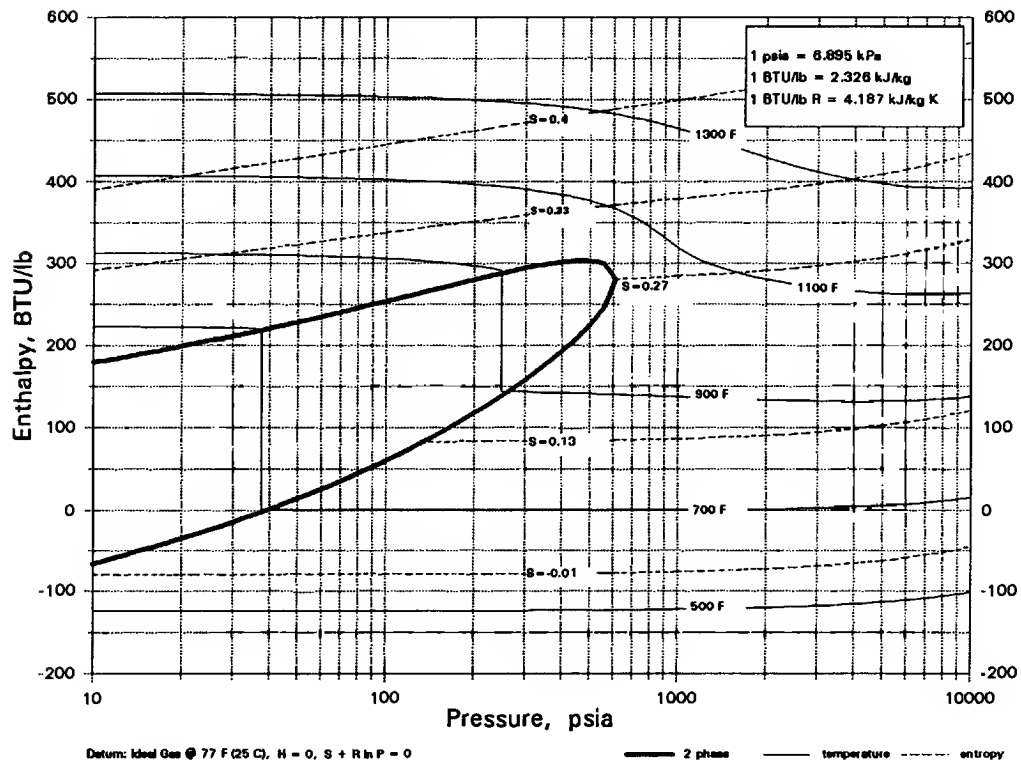
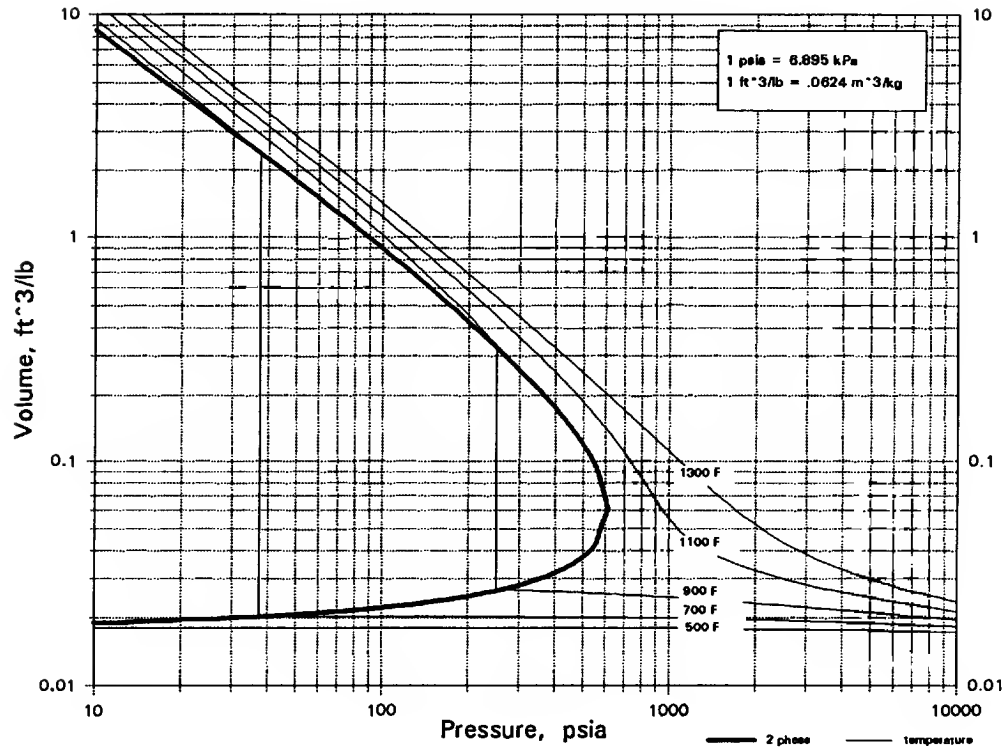


C5H6O4
CITRACONIC ACID



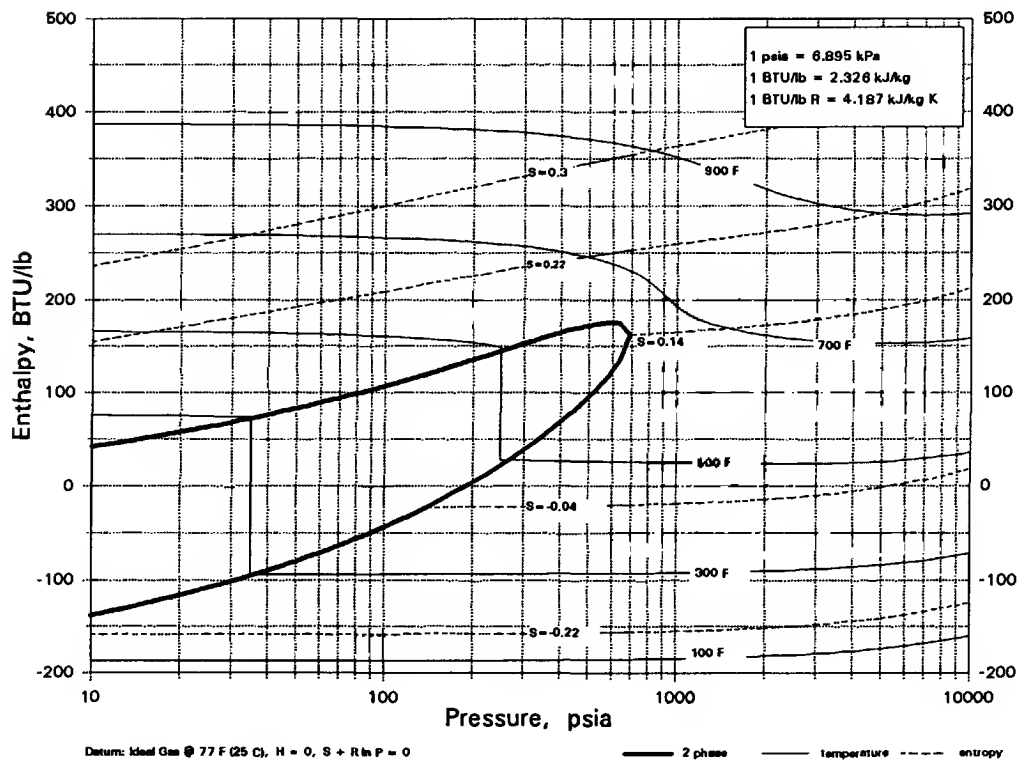
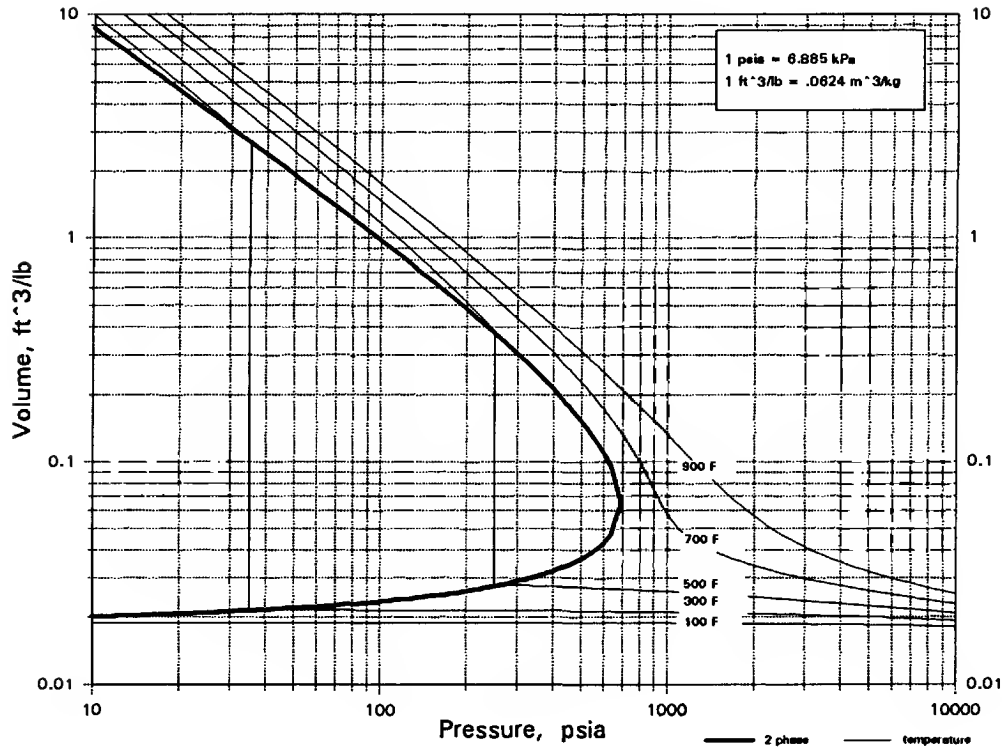
C5H6O4

ITACONIC ACID



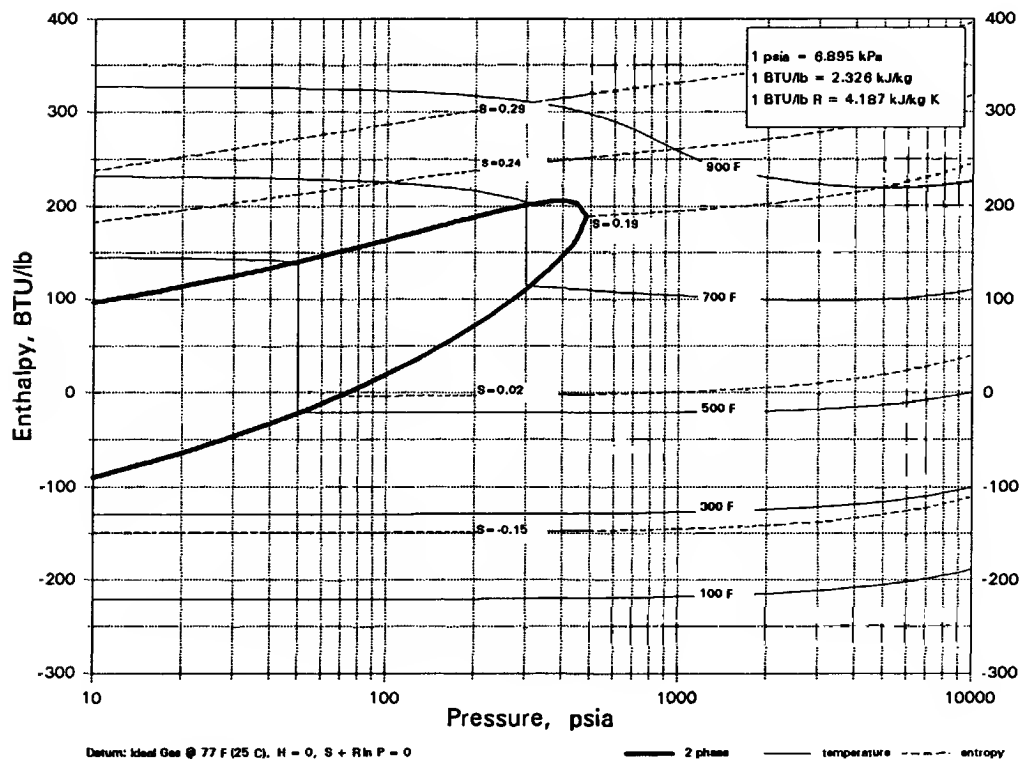
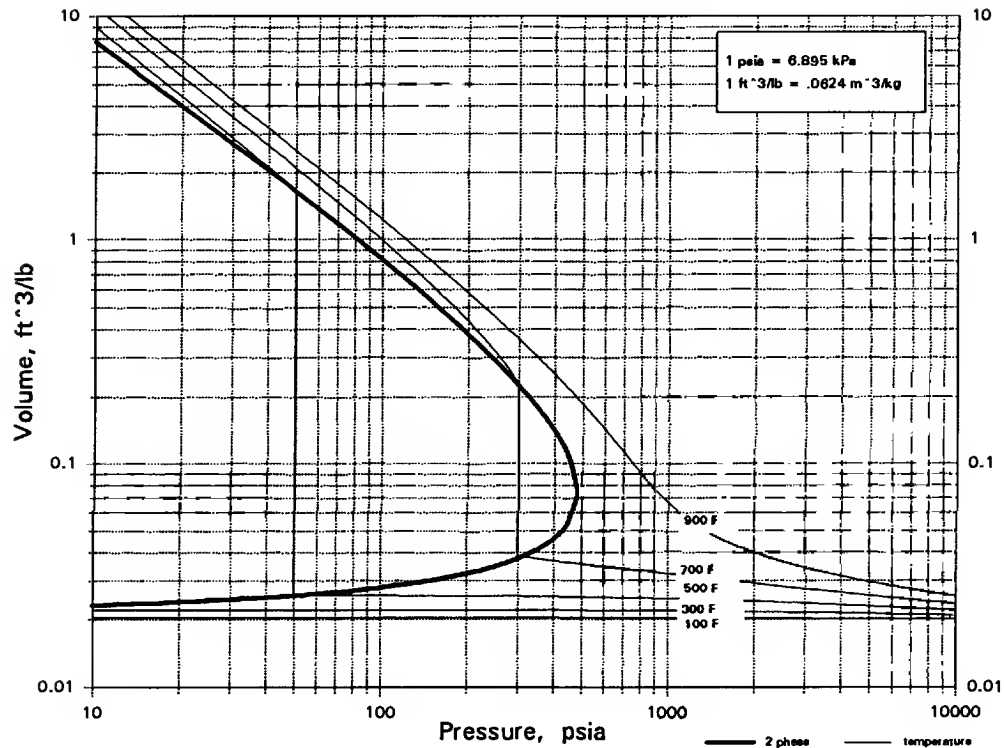
C5H7N

N-METHYLPYRROLE



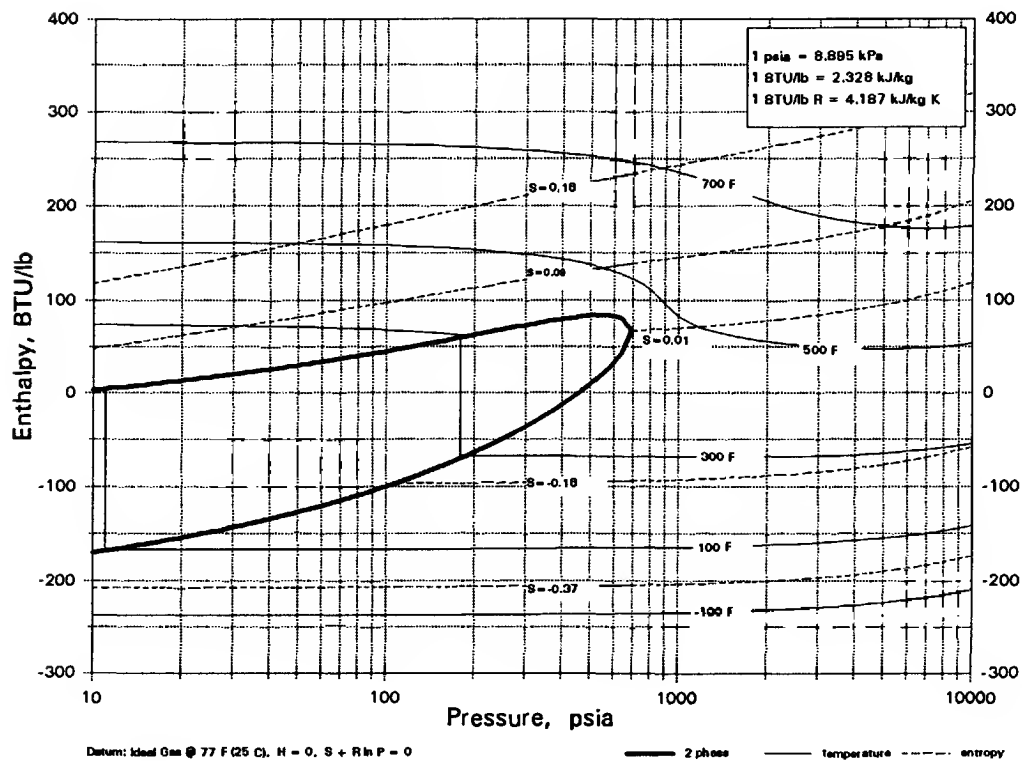
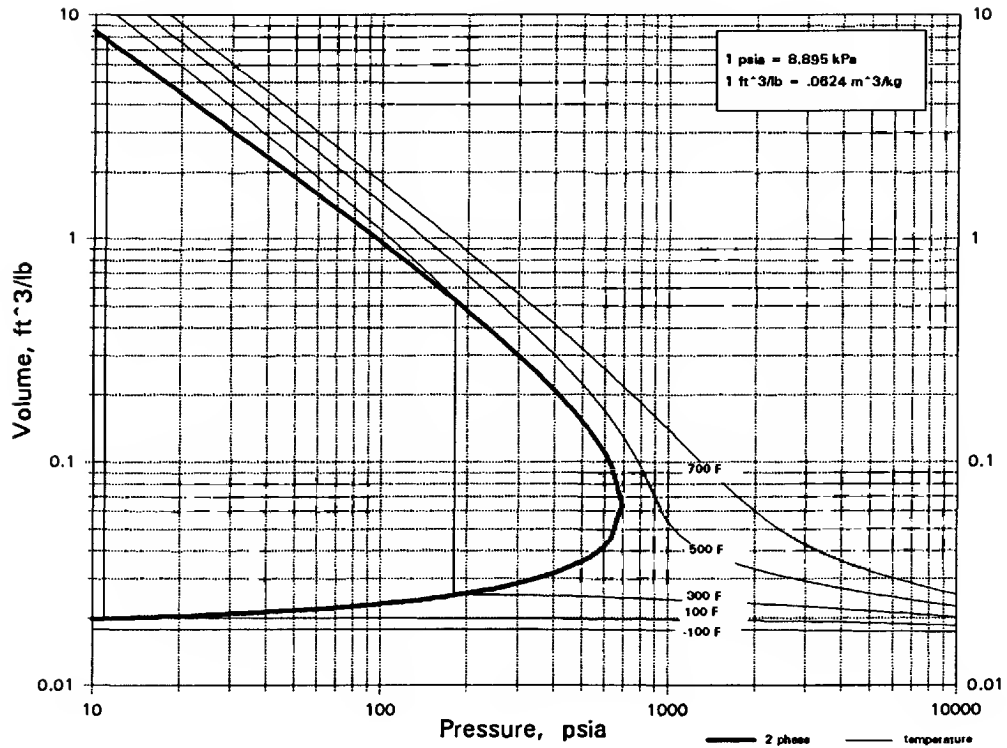
C5H7NO2

ETHYL CYANOACETATE



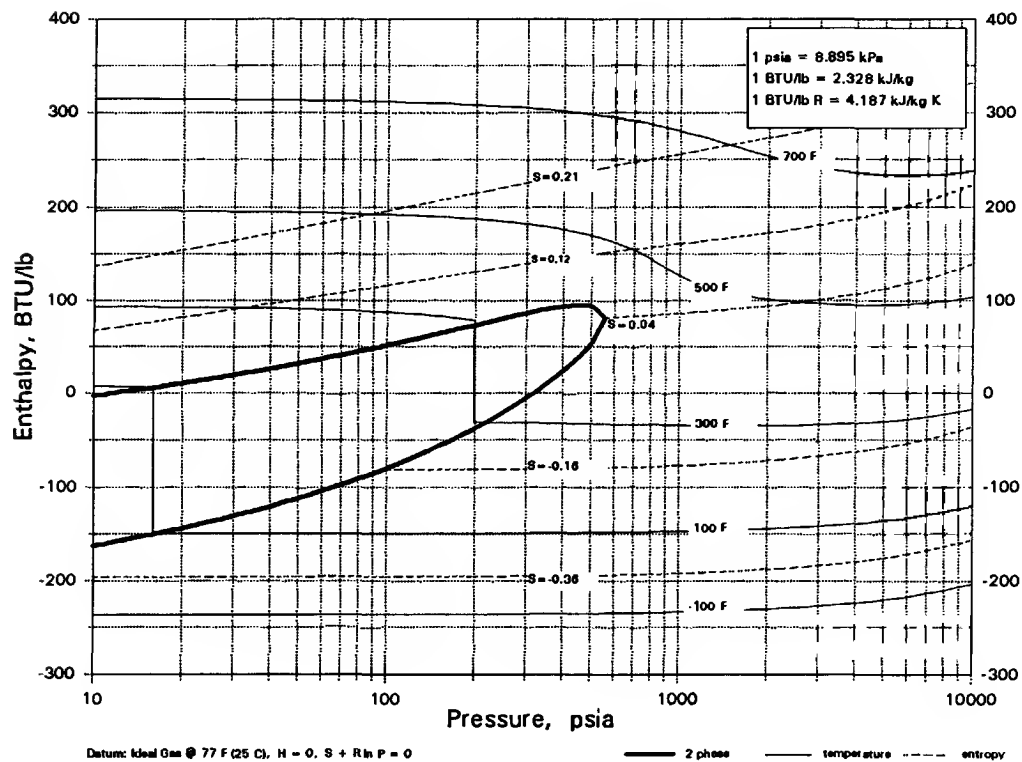
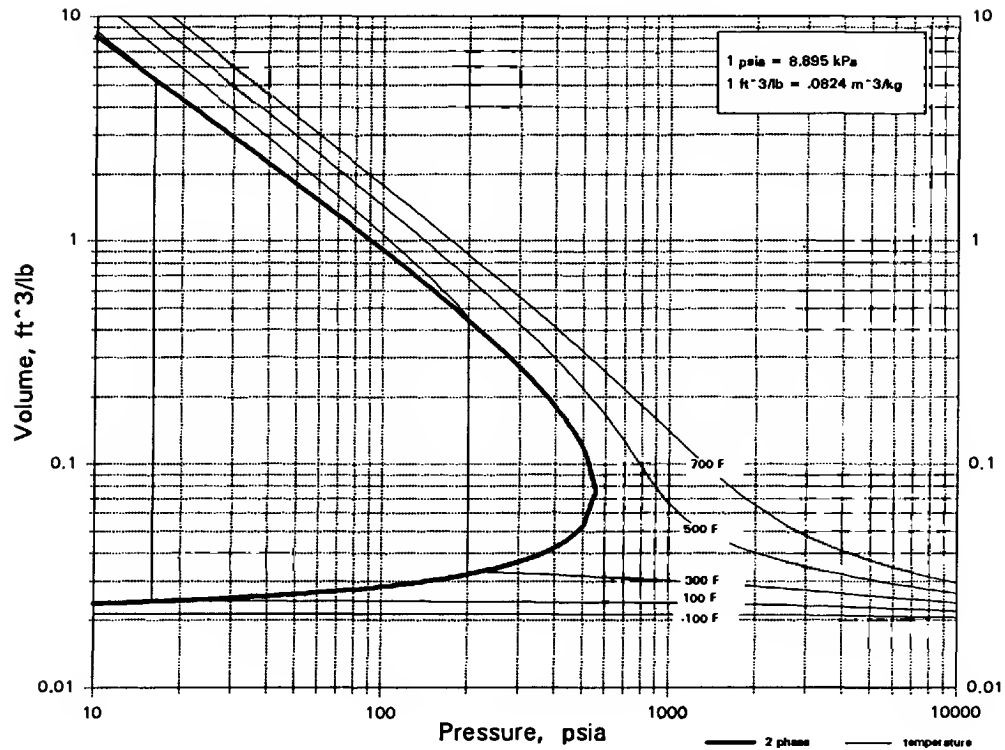
C5H8

CYCLOPENTENE

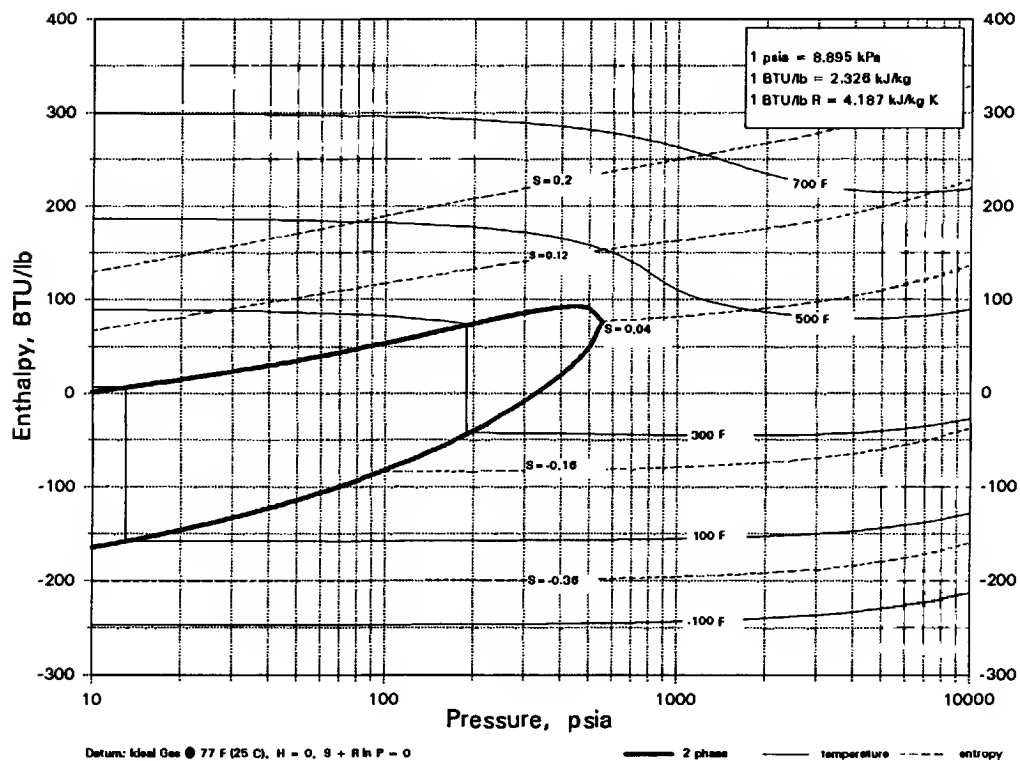
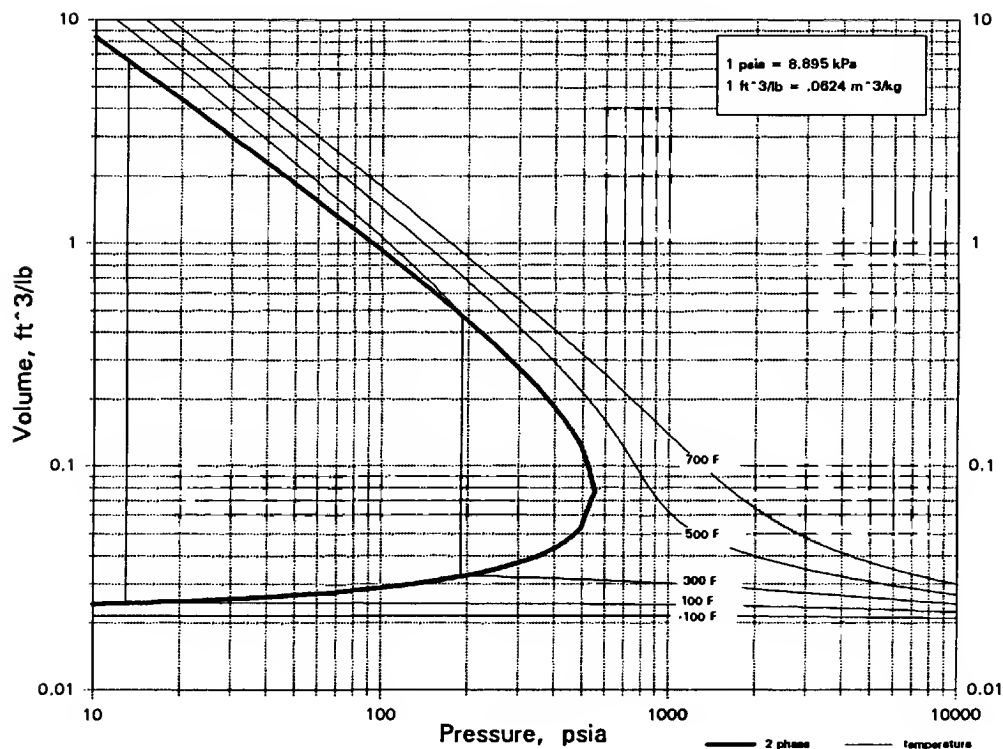


C5H8

ISOPRENE

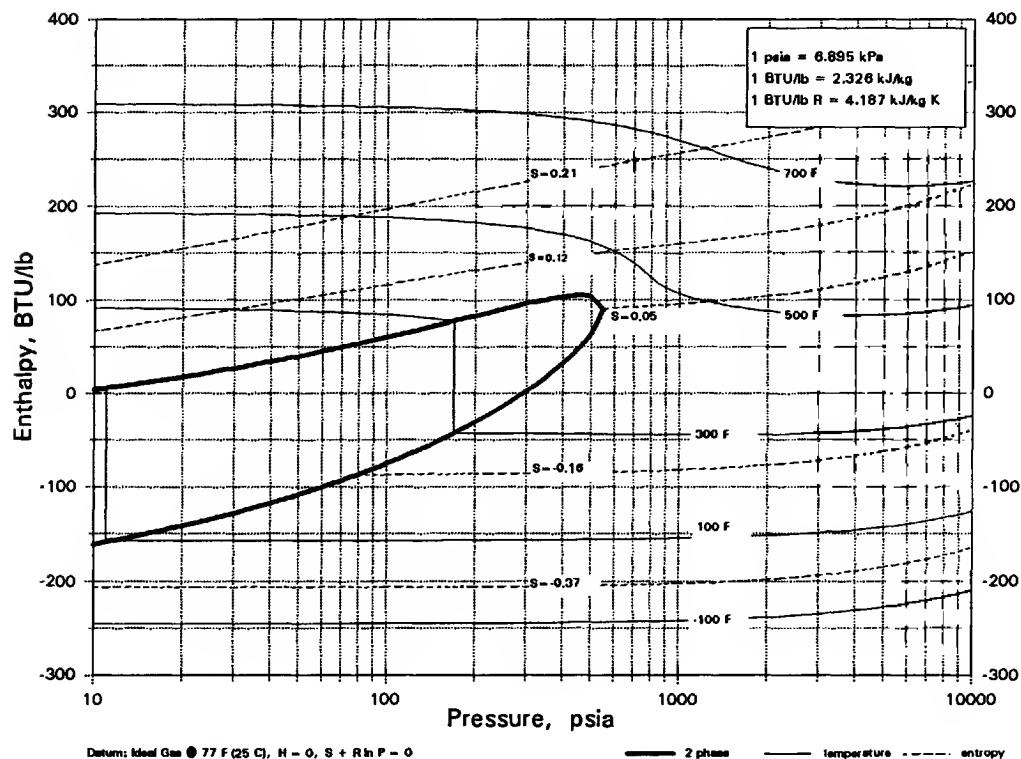
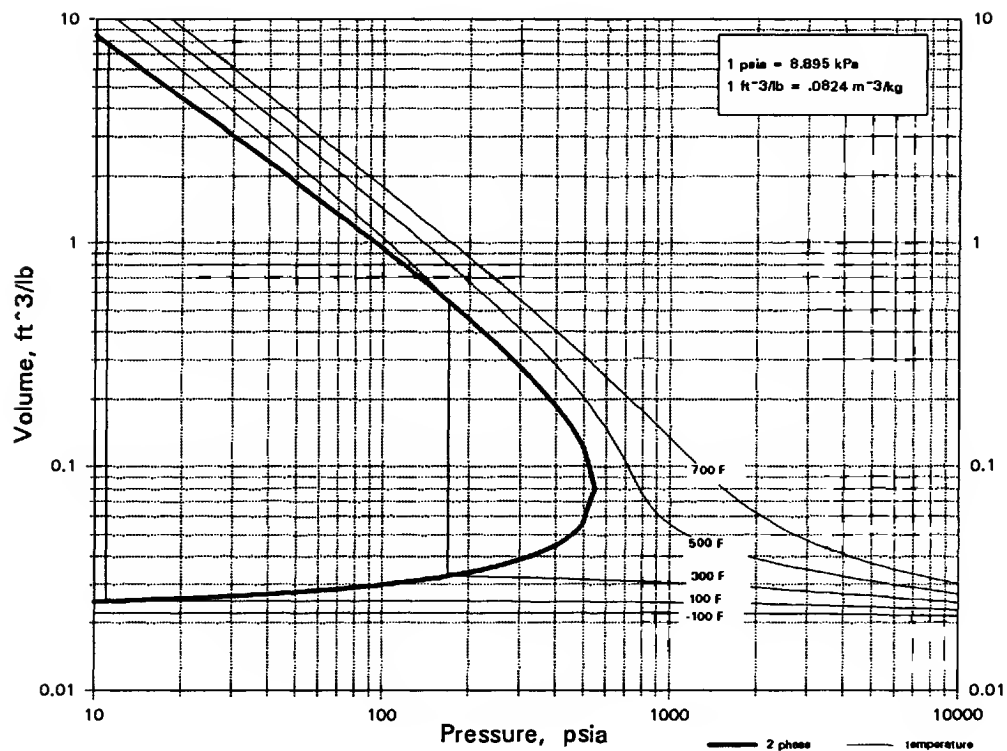


C5H8
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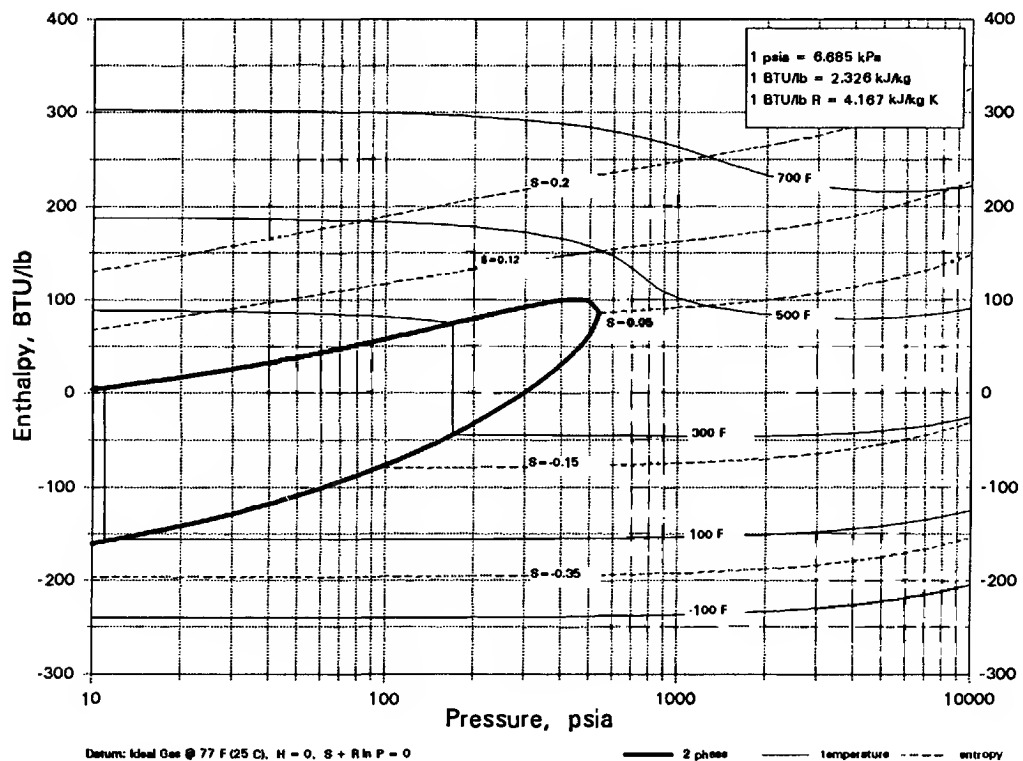
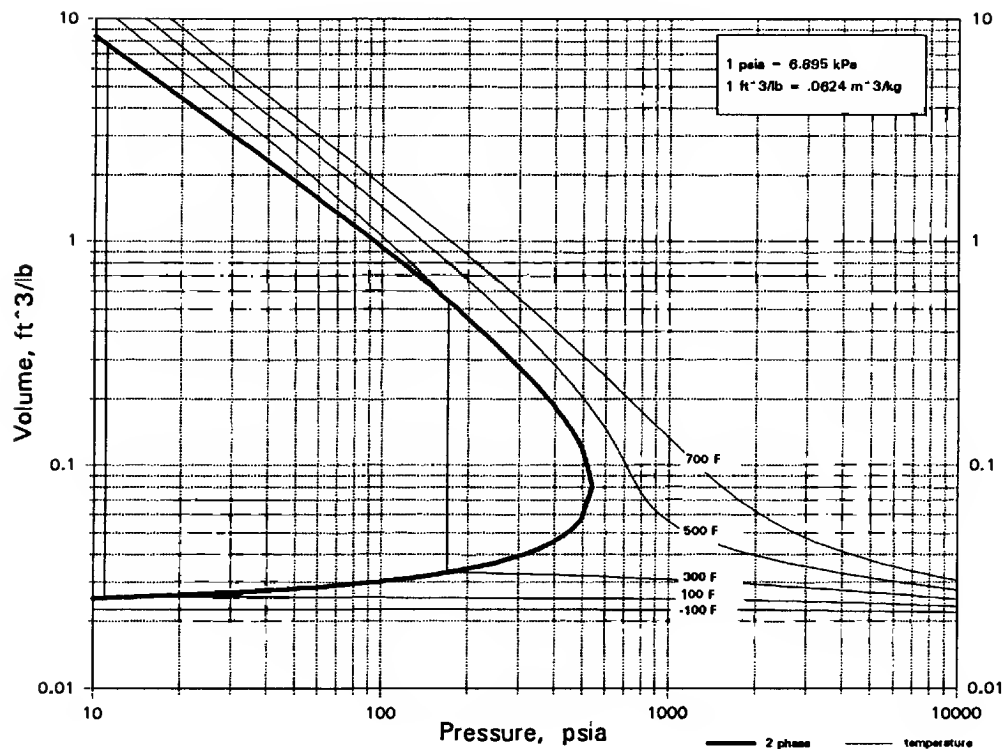


C5H8

1-2-PENTADIENE

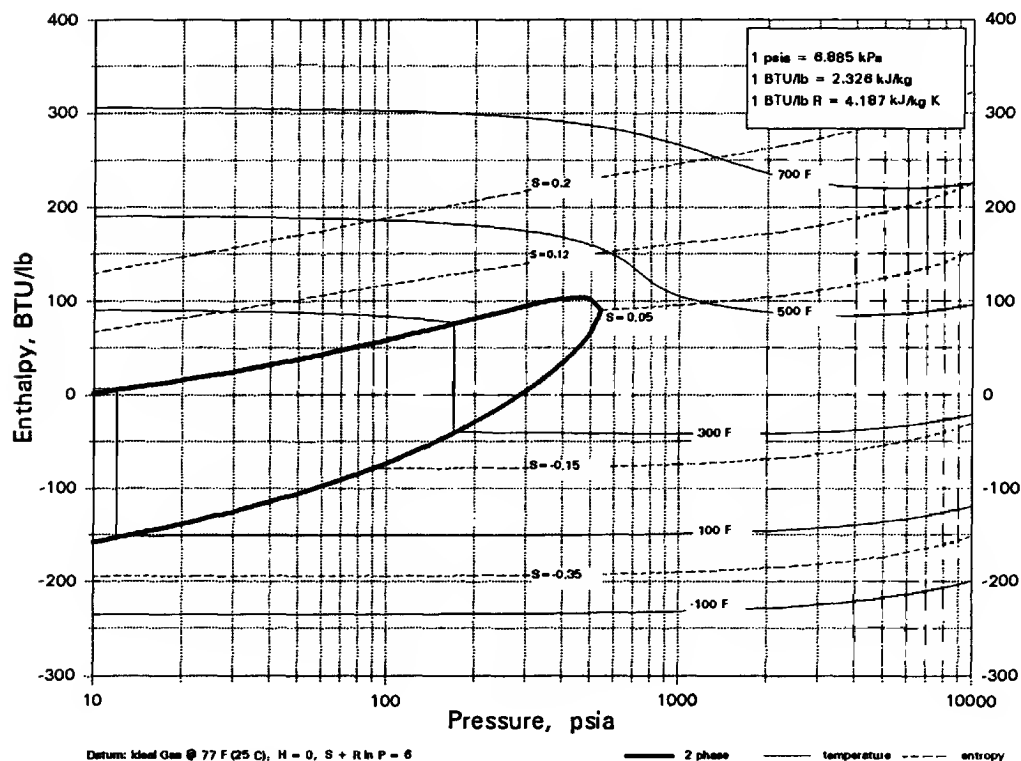
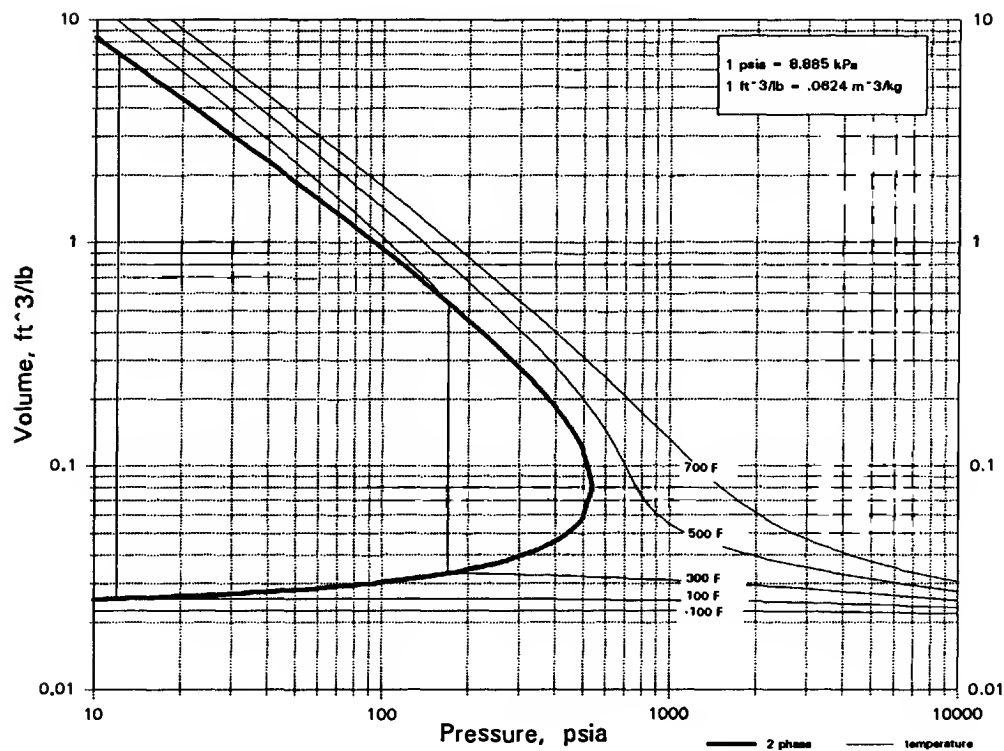


C5H8
cis-1-3-PENTADIENE



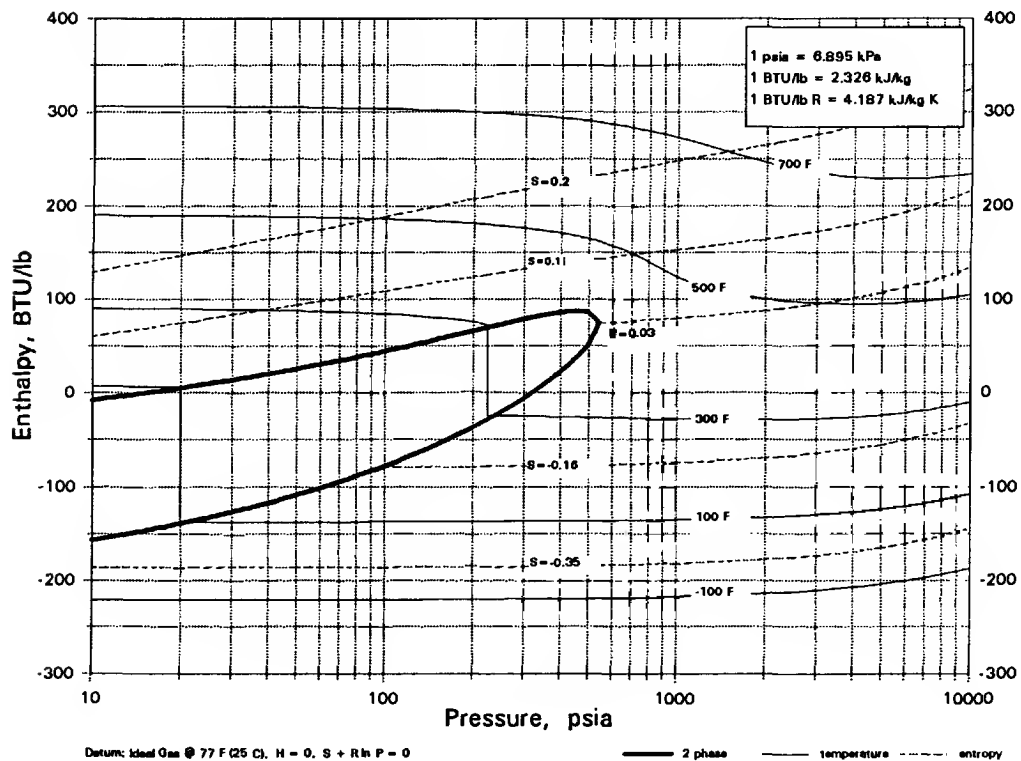
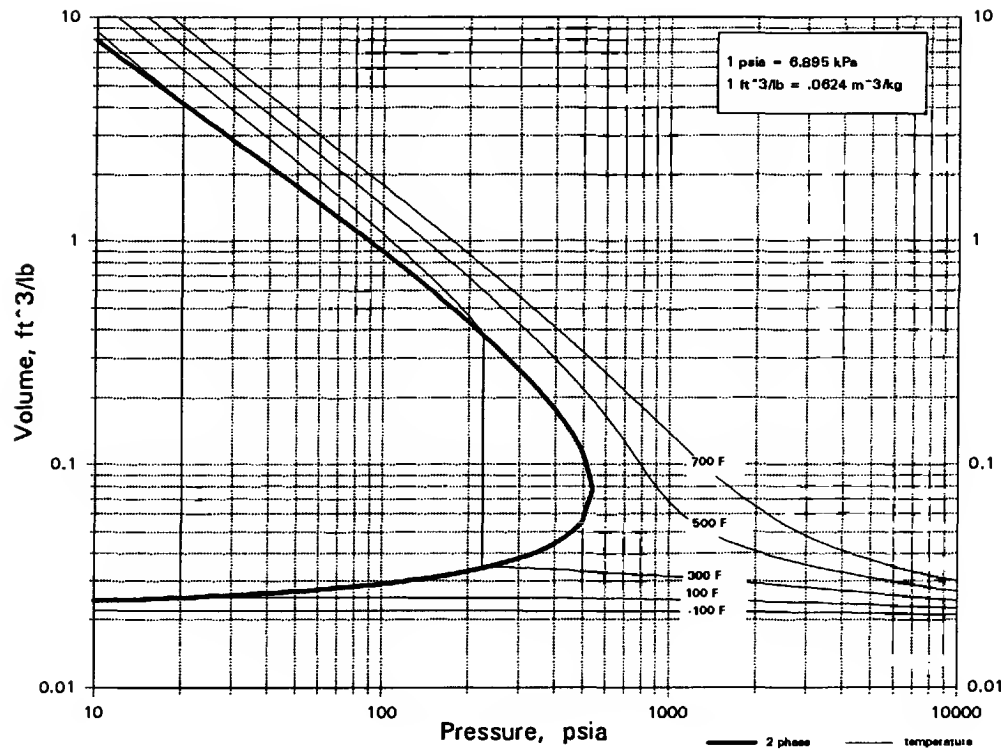
C5H8

trans-1-3-PENTADIENE



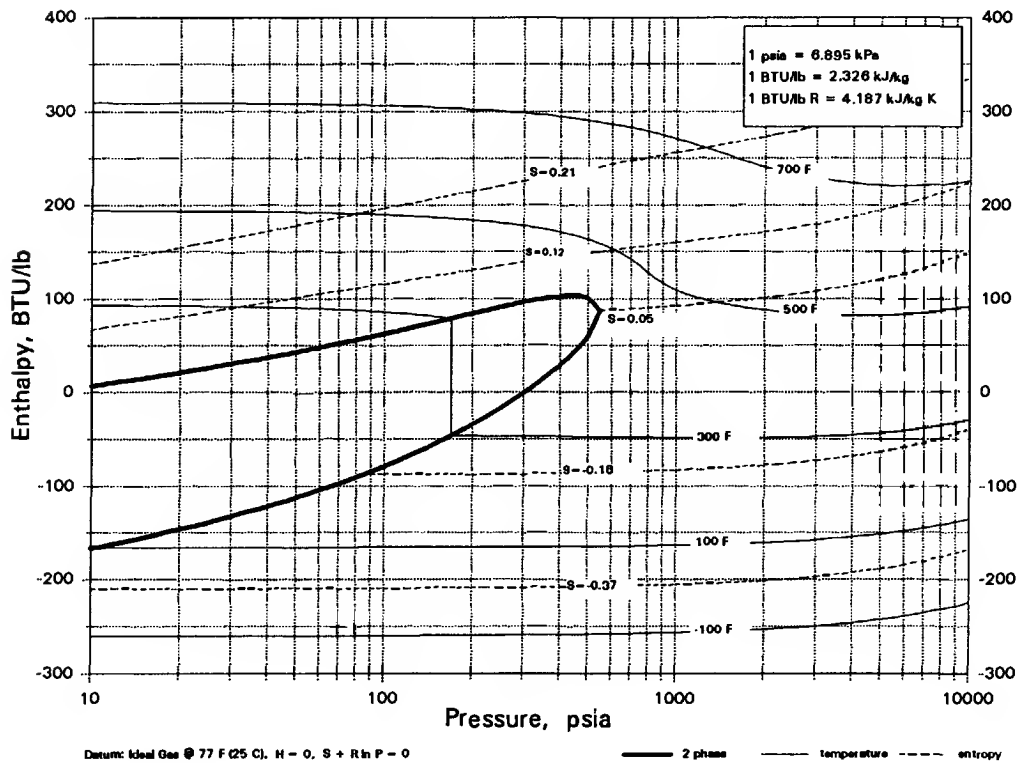
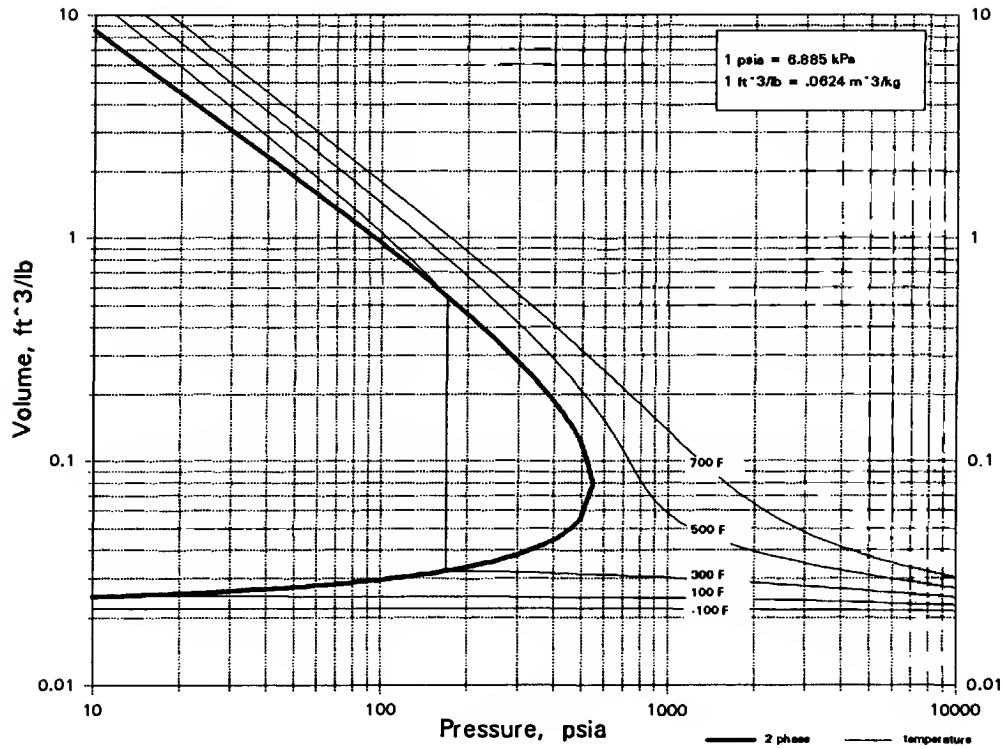
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1-4-PENTADIENE



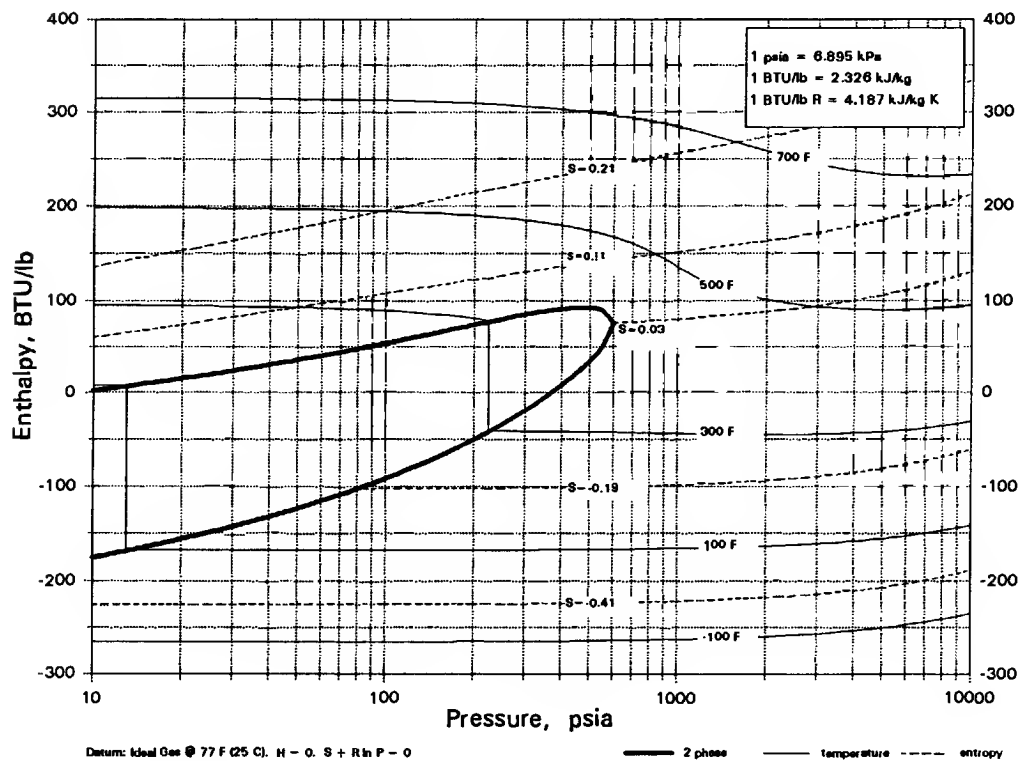
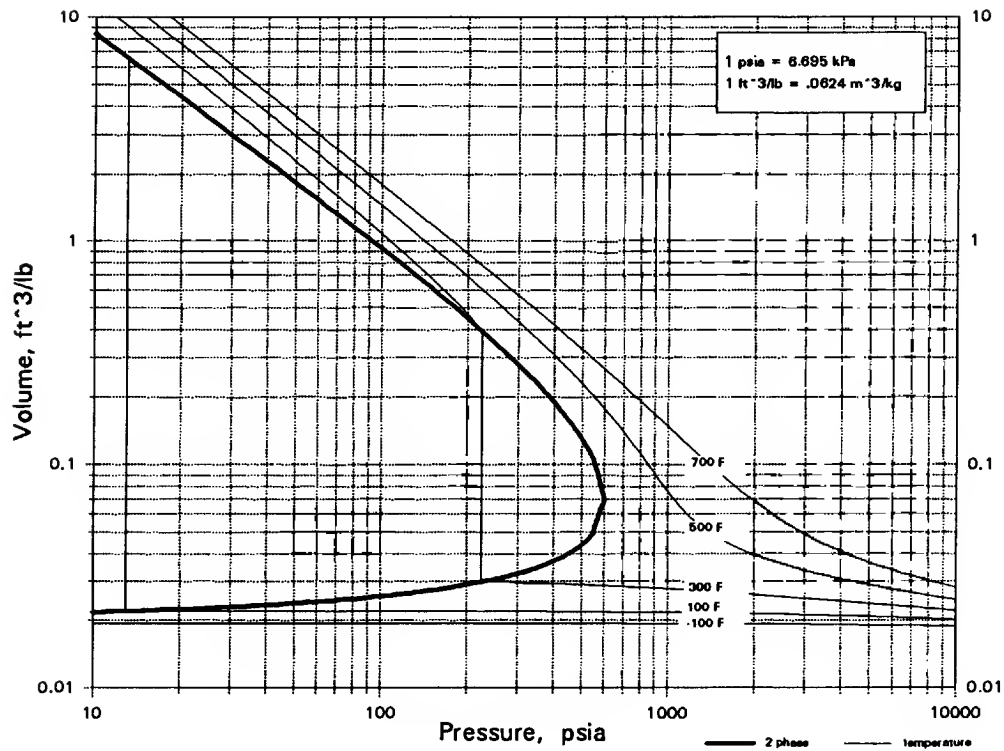
C5H8

2-3-PENTADIENE



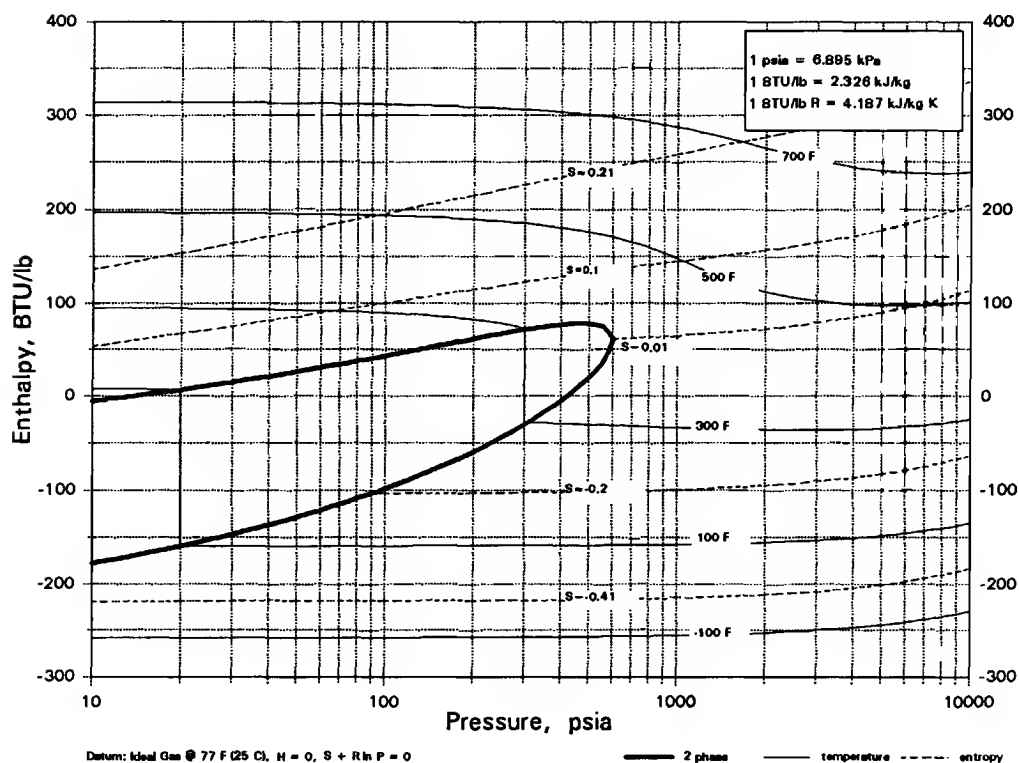
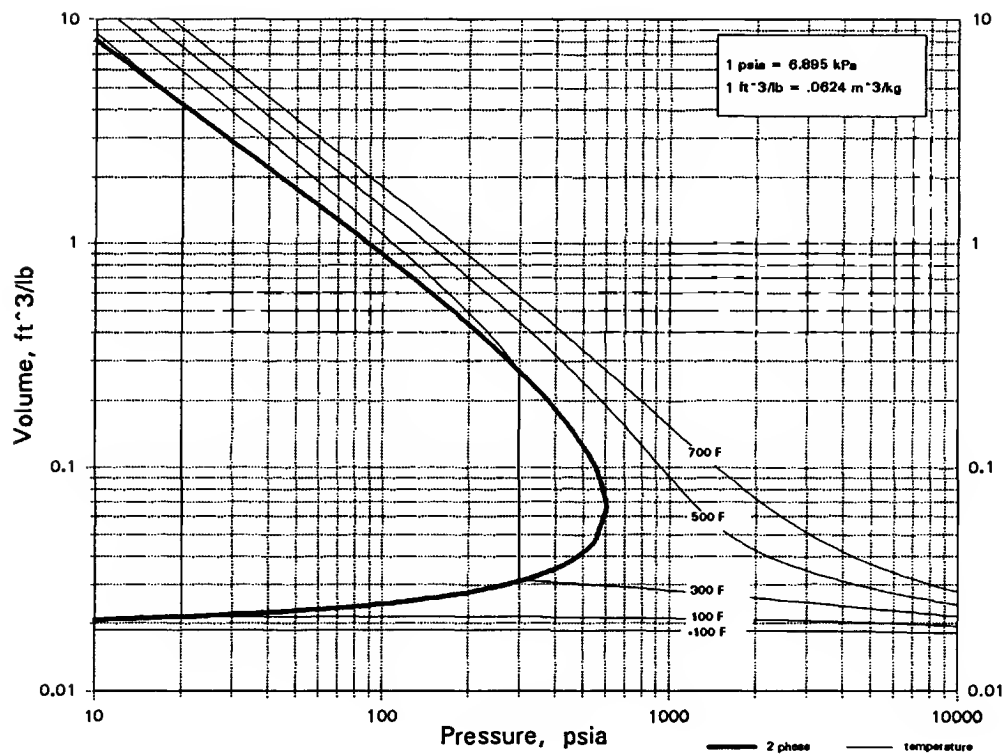
C5H8

1-PENTYNE

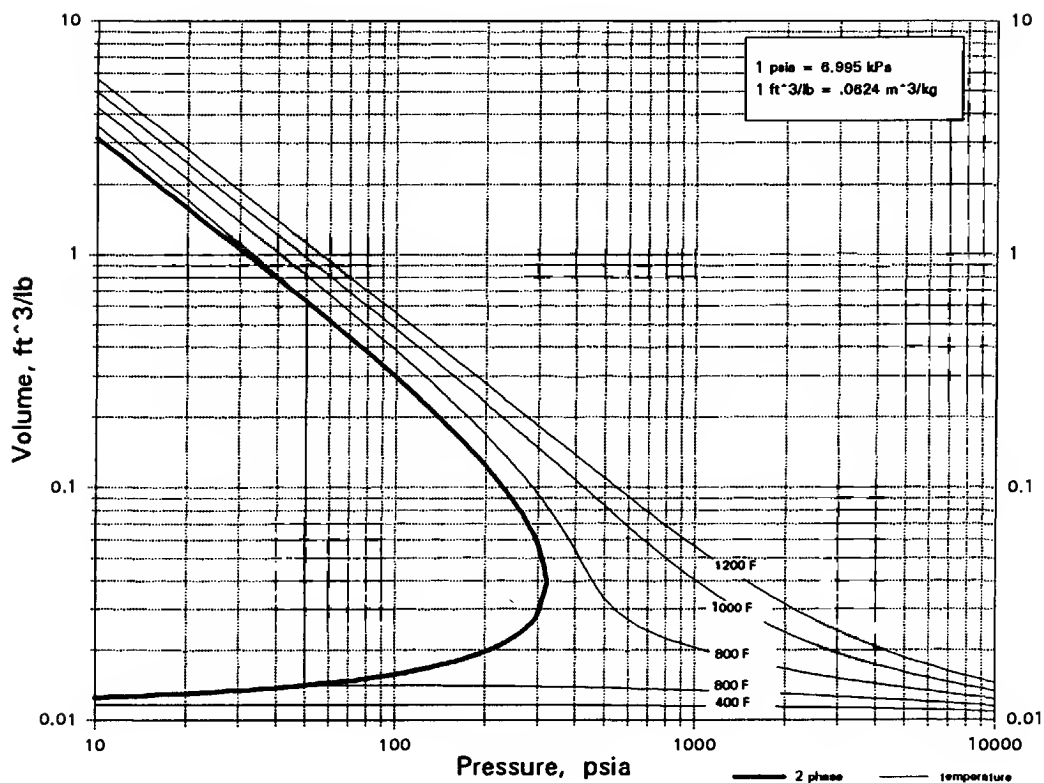


C5H8

3-METHYL-1-BUTYNE



C5H8N4O12 PENTAERYTHRITOL TETRANITRATE



1. Boiling Point, K..... 543.00

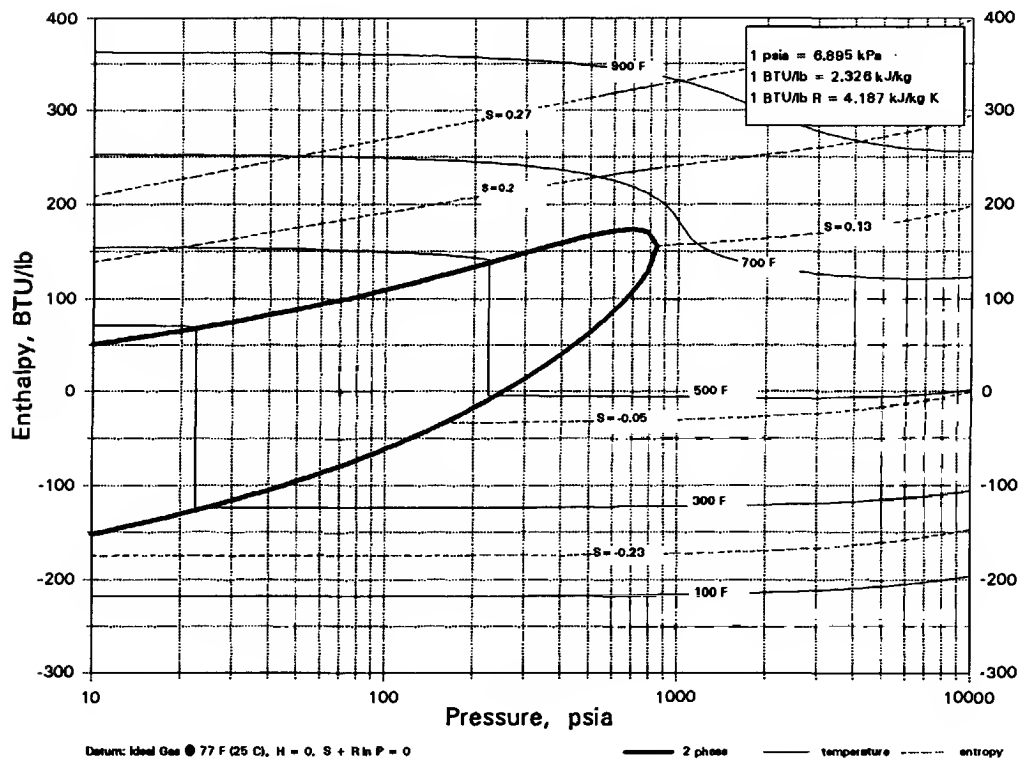
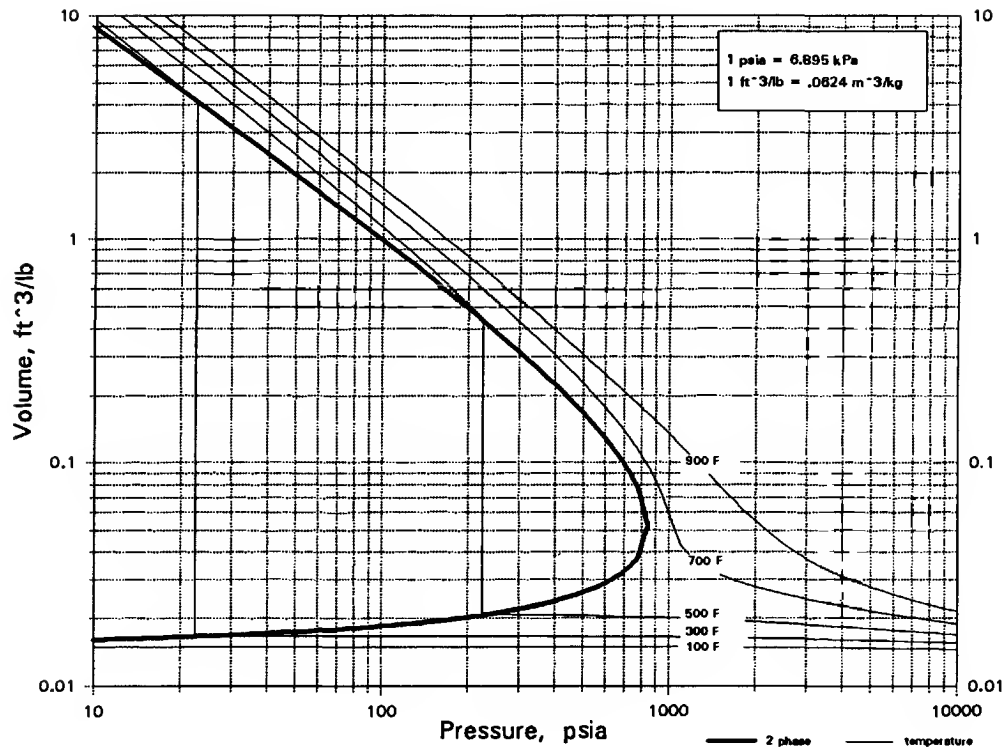
2. Critical Temperature, K.... 676.00

3. Critical Pressure, atm..... 22.11

Heat capacity data are not available.

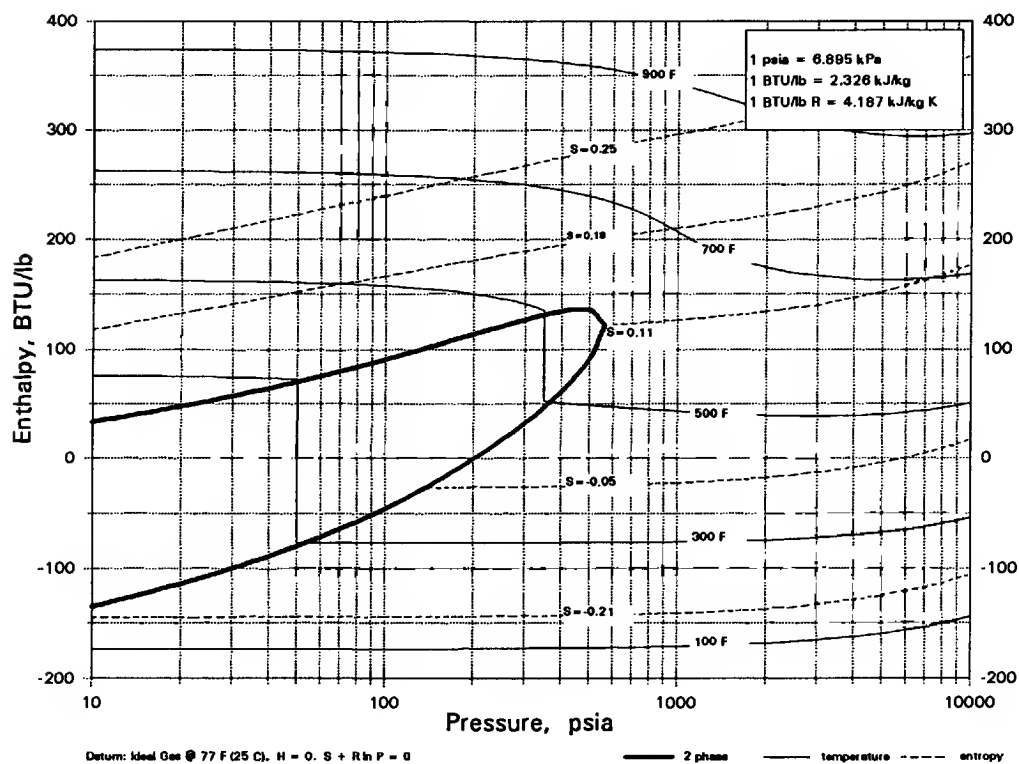
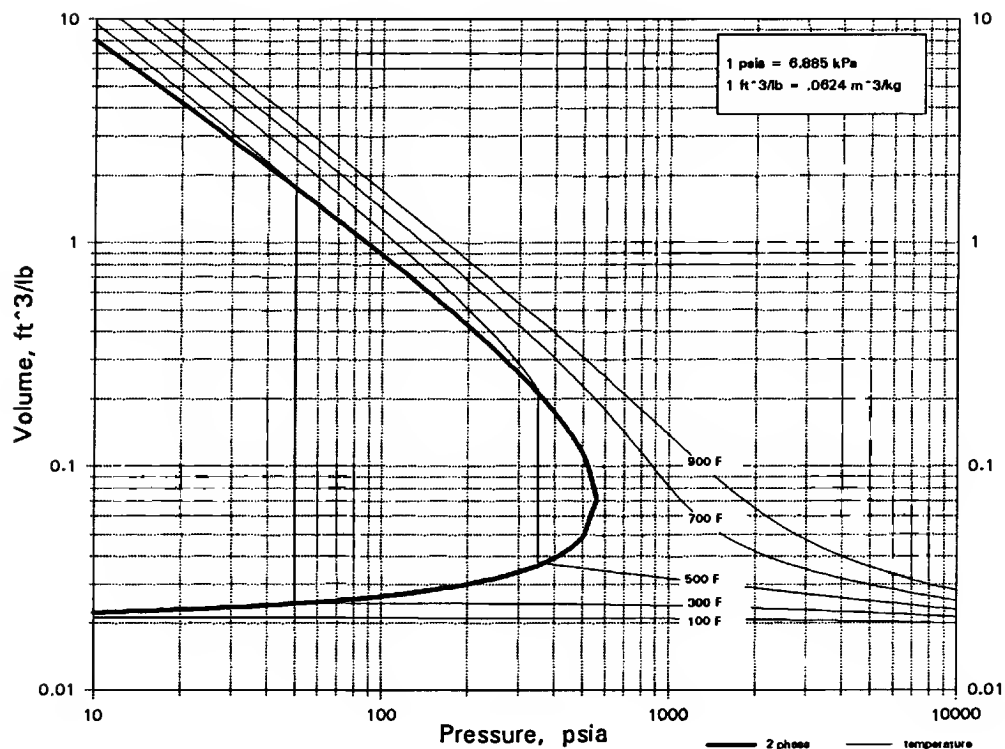
C5H8O

CYCLOPENTANONE



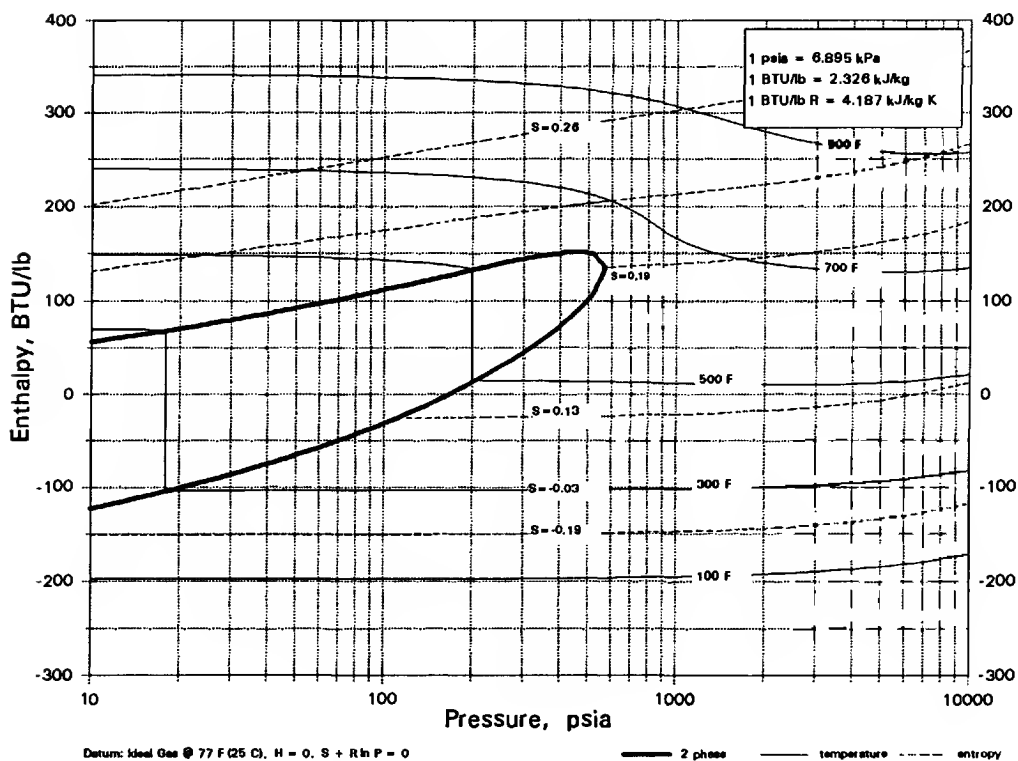
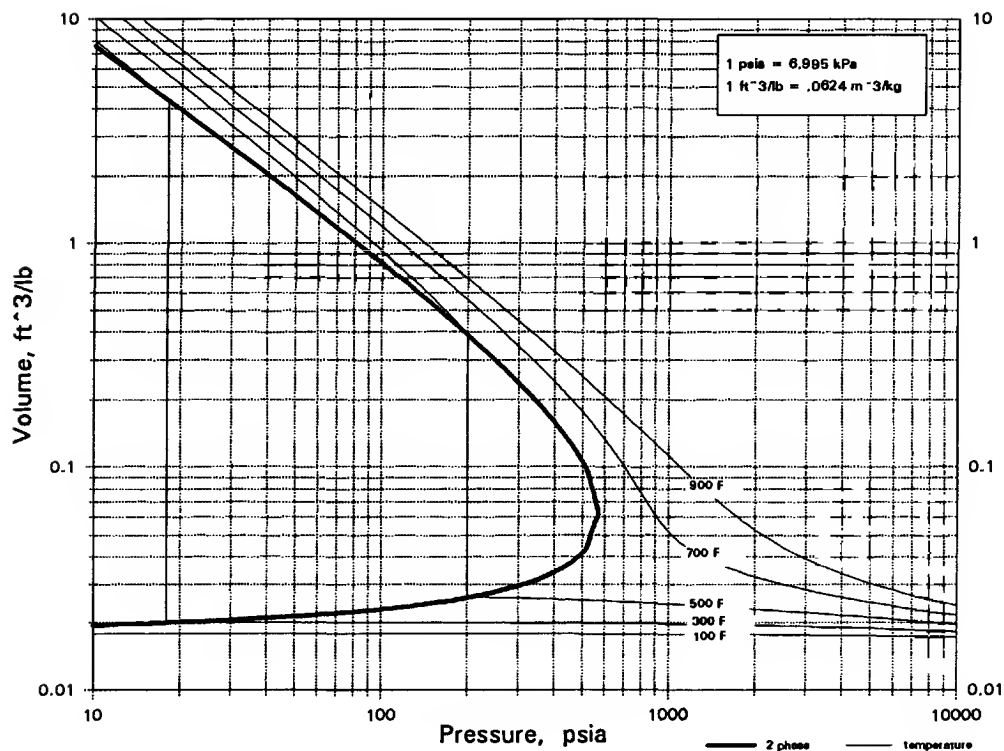
C5H8O

METHYL ISOPROPENYL KETONE



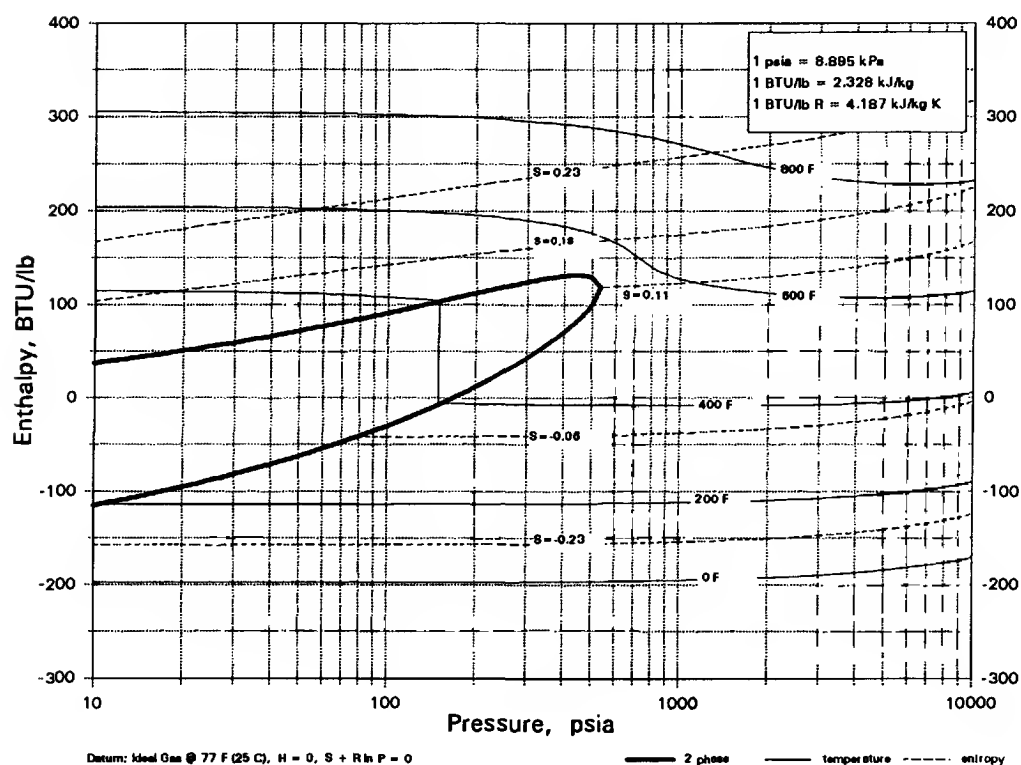
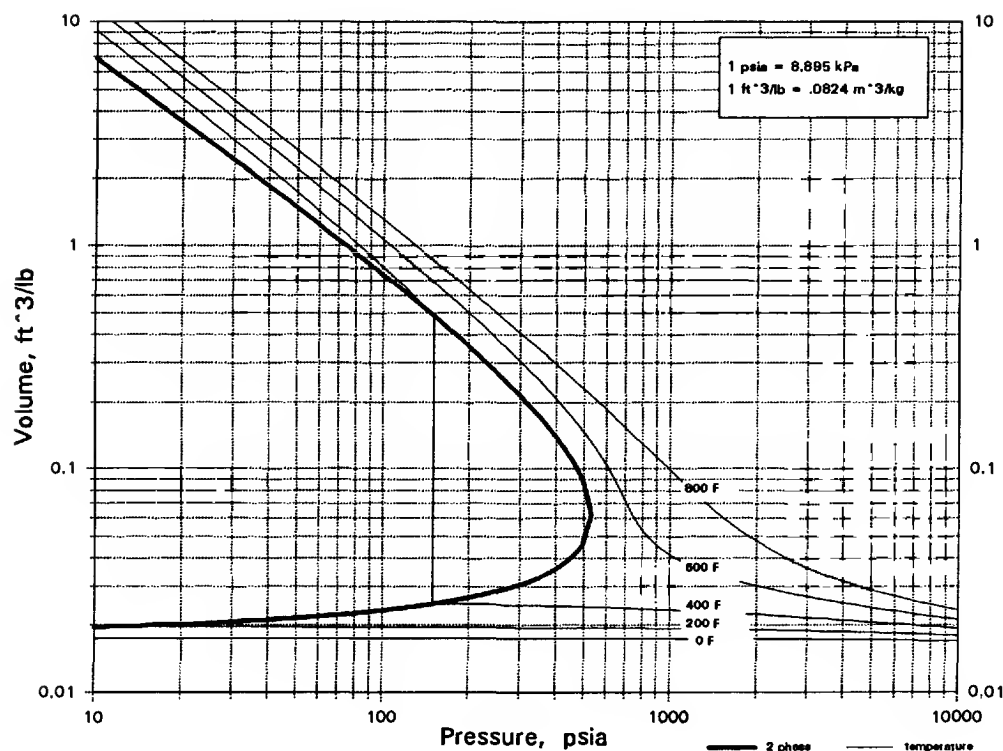
C5H8O2

ACETYLACETONE



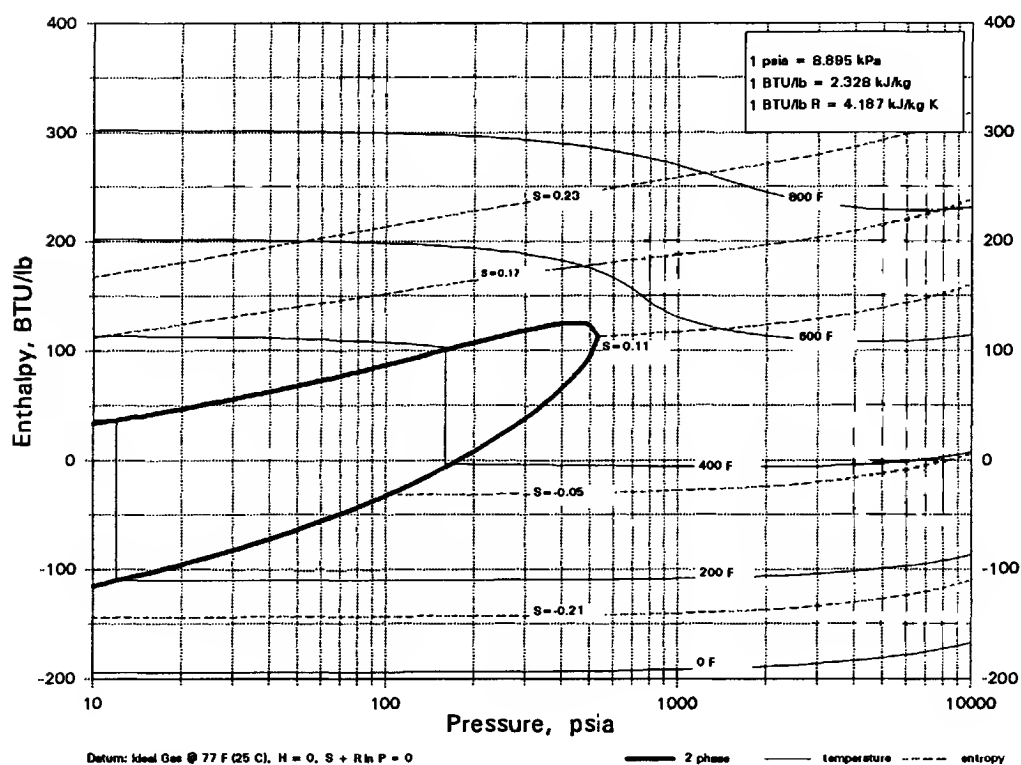
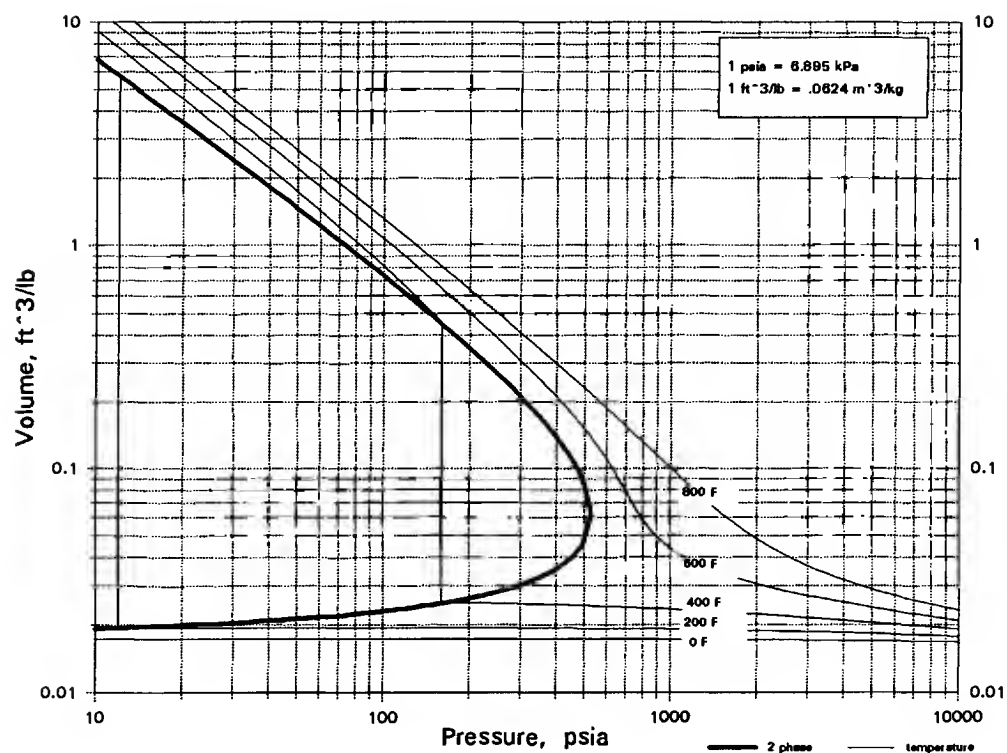
C5H8O2

ALLYL ACETATE



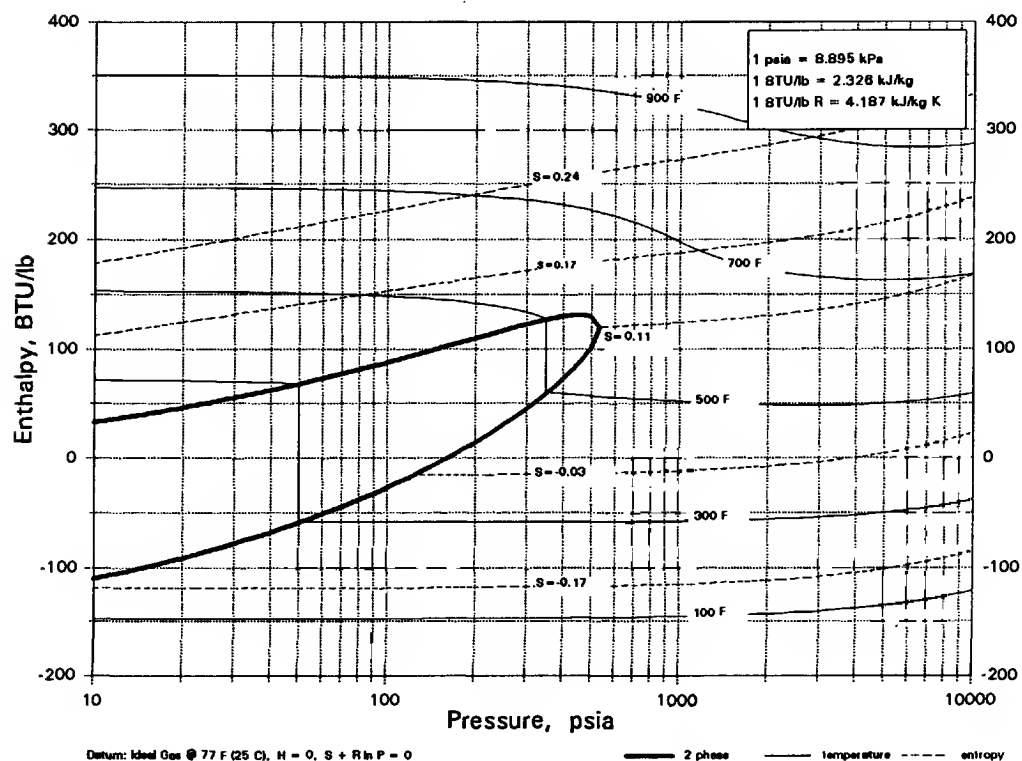
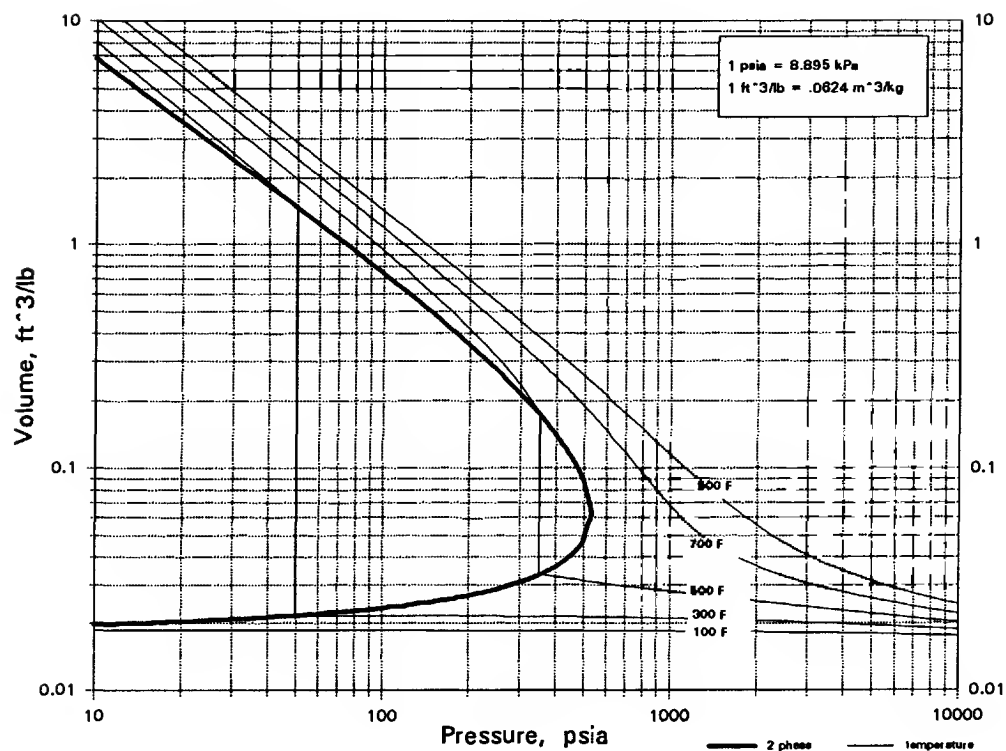
C5H8O2

ETHYL ACRYLATE



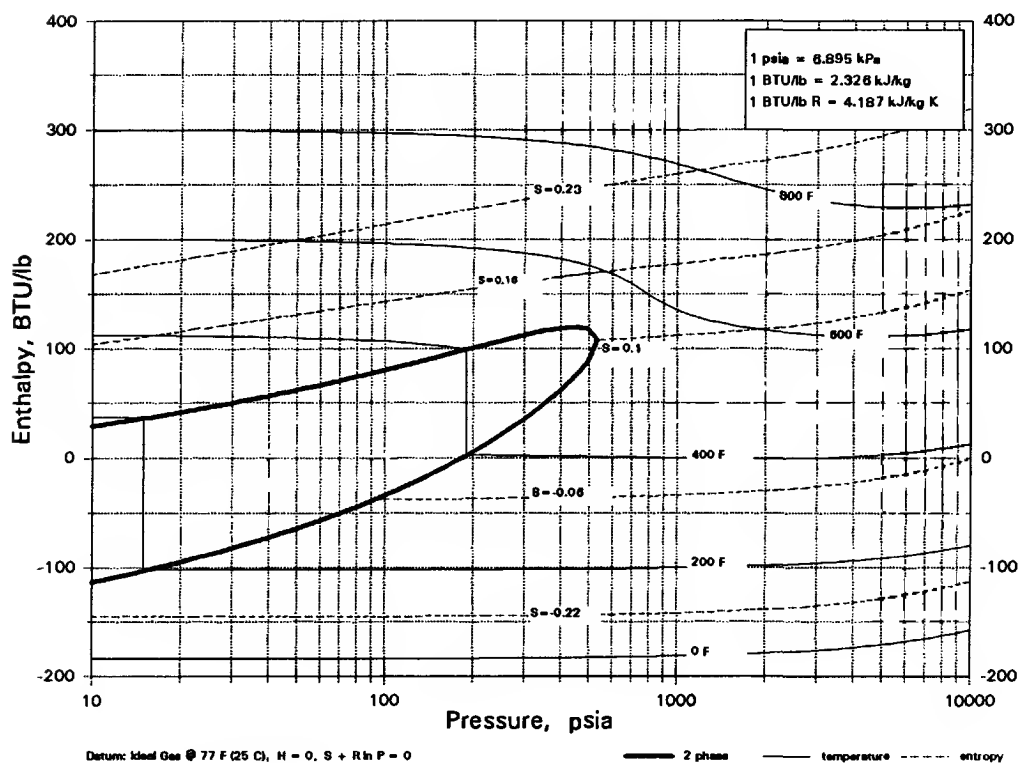
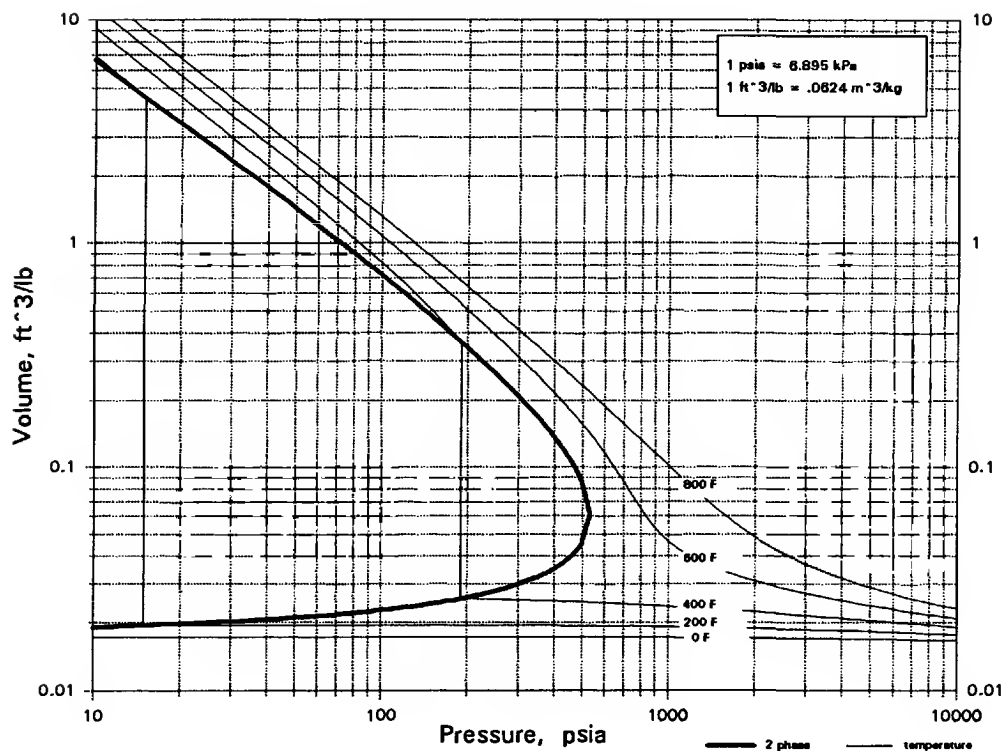
C5H8O2

METHYL METHACRYLATE



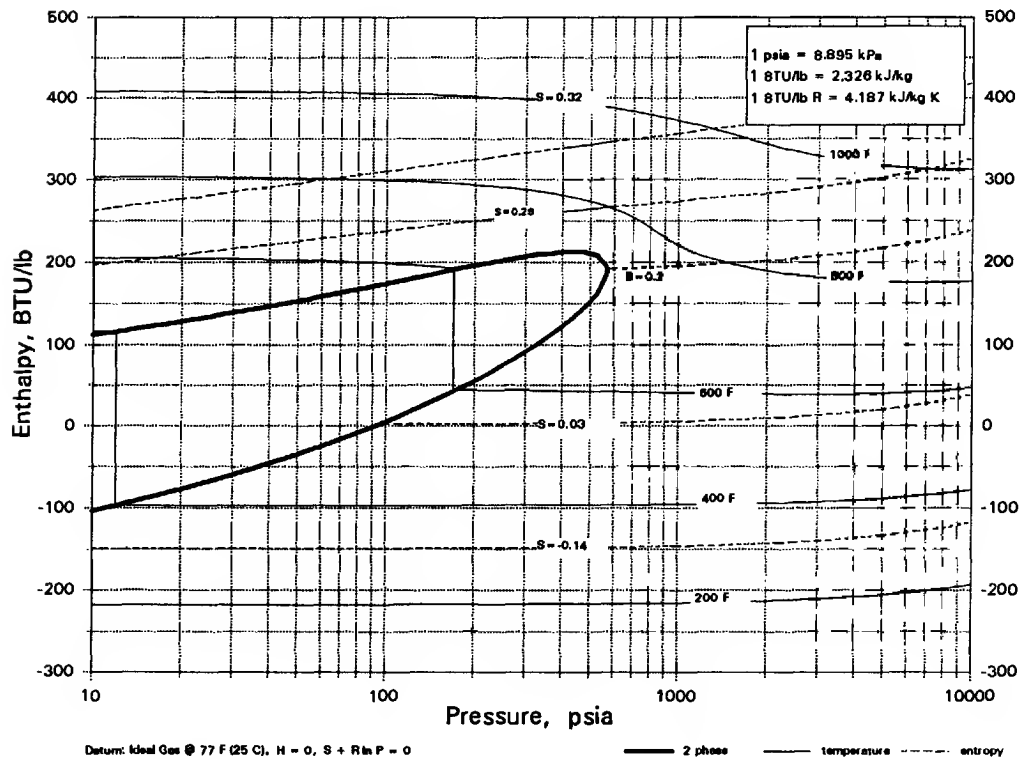
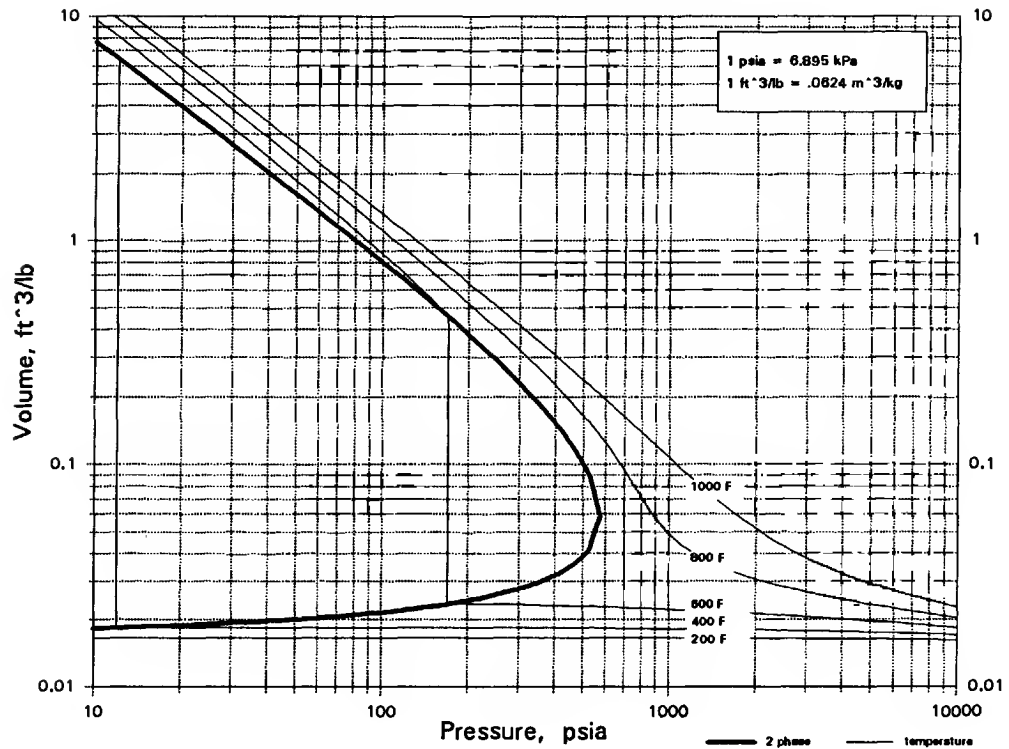
C5H8O2

VINYL PROPIONATE



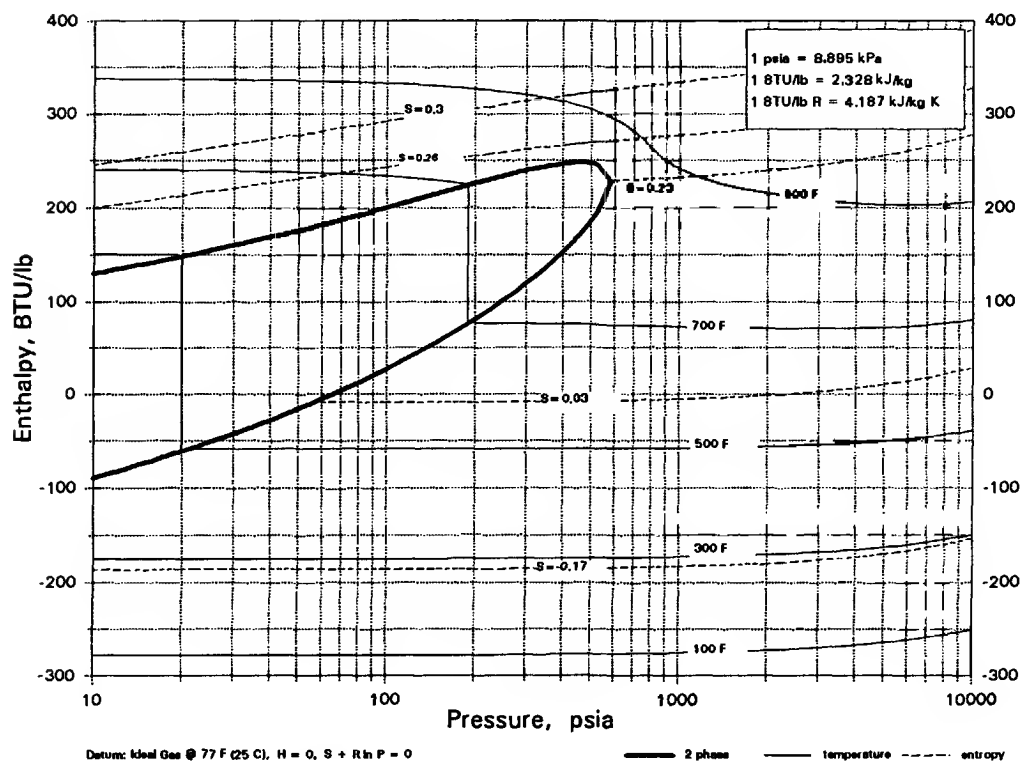
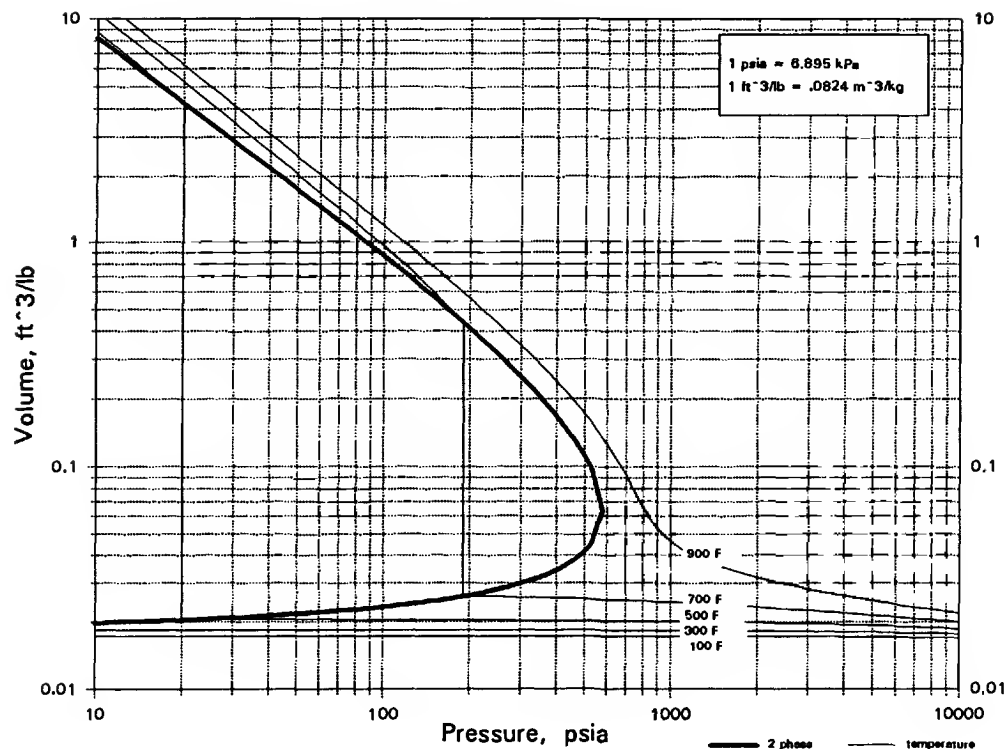
C5H8O3

2-HYDROXYETHYL ACRYLATE



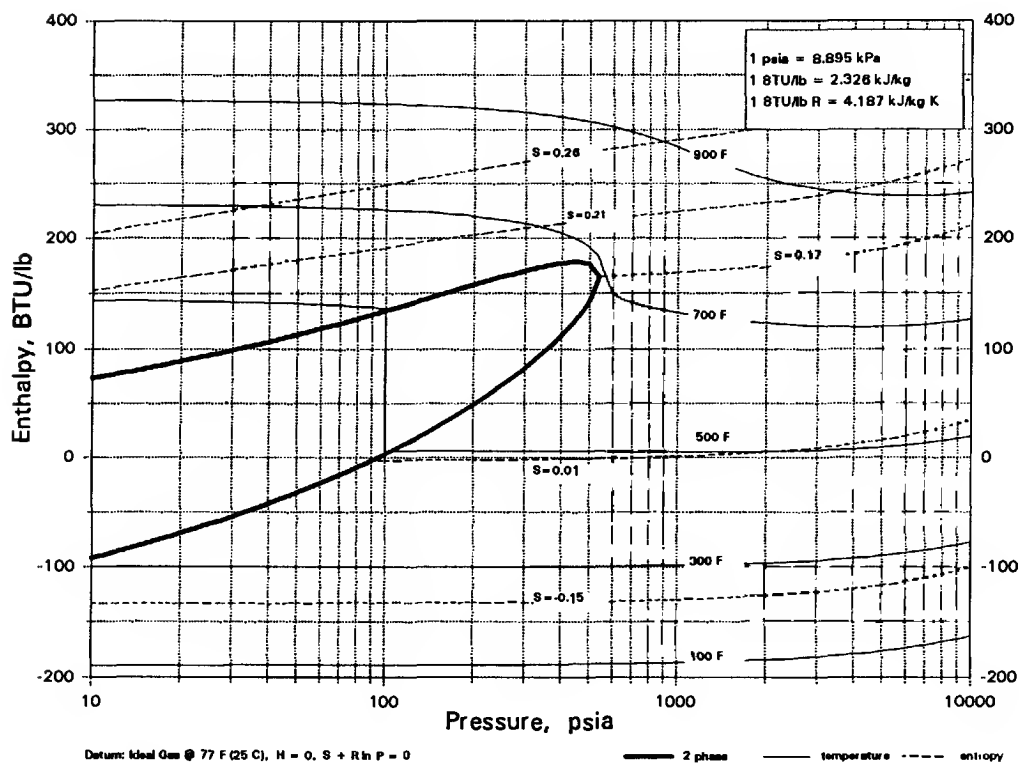
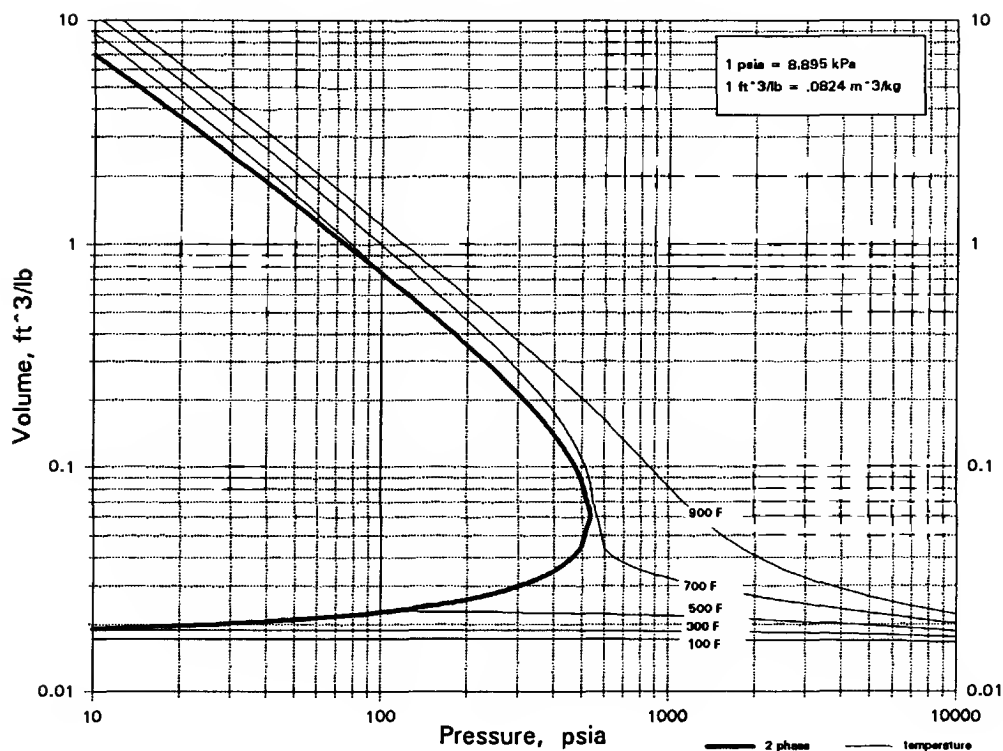
C5H8O3

LEVULINIC ACID



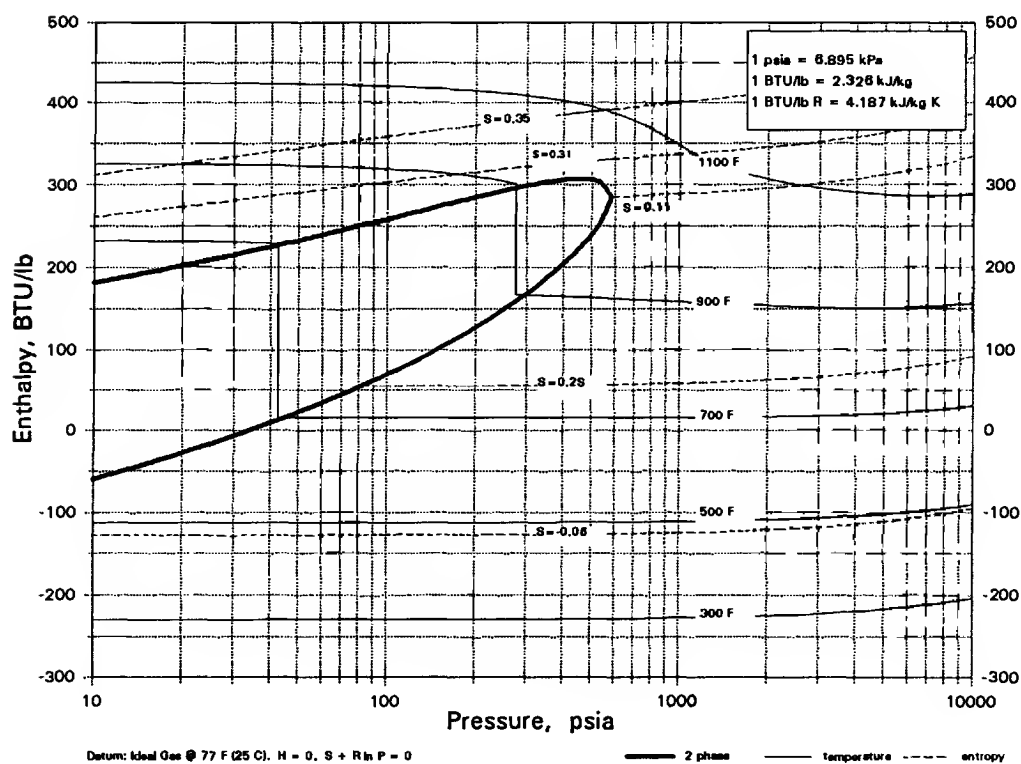
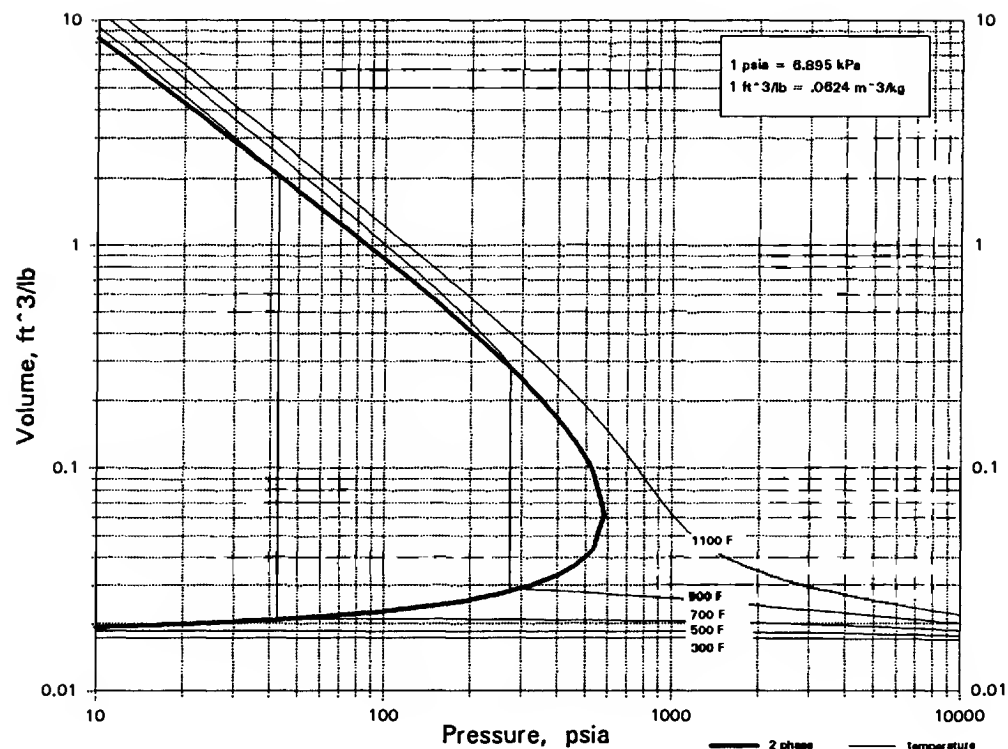
C5H8O3

METHYL ACETOACETATE



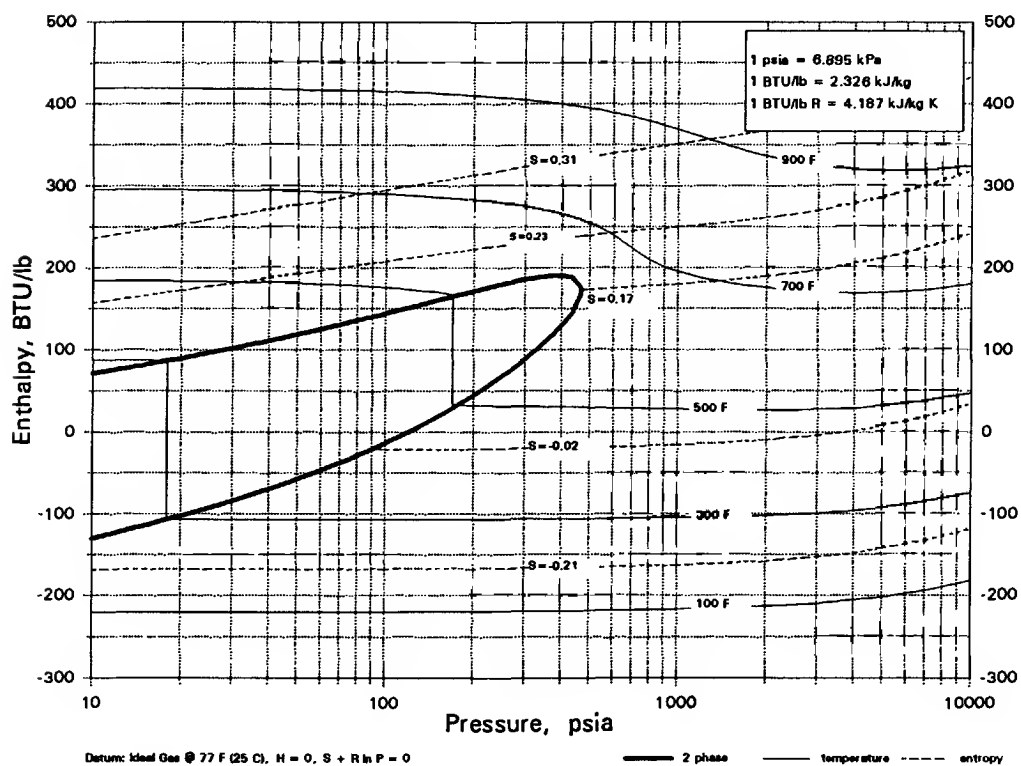
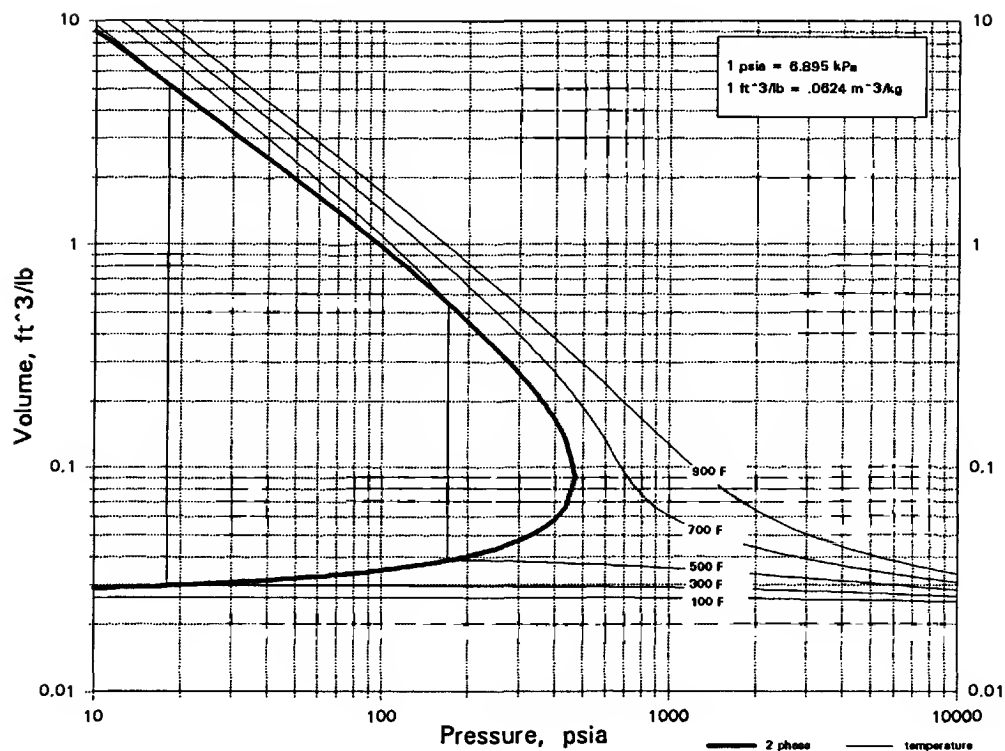
C5H8O4

GLUTARIC ACID



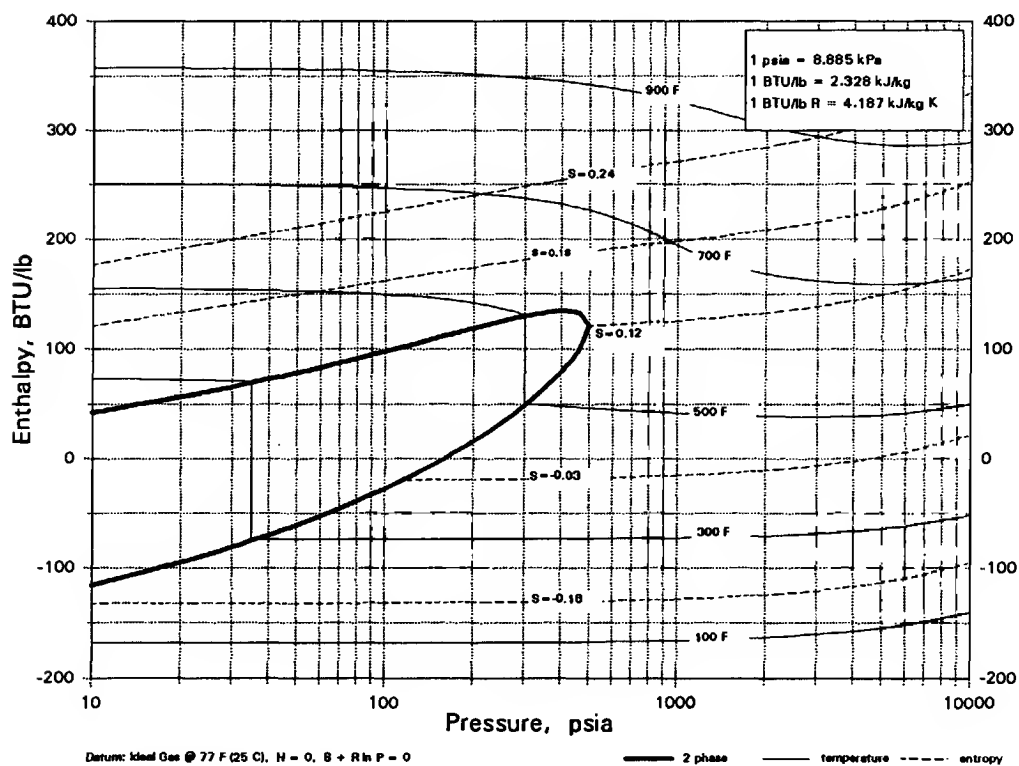
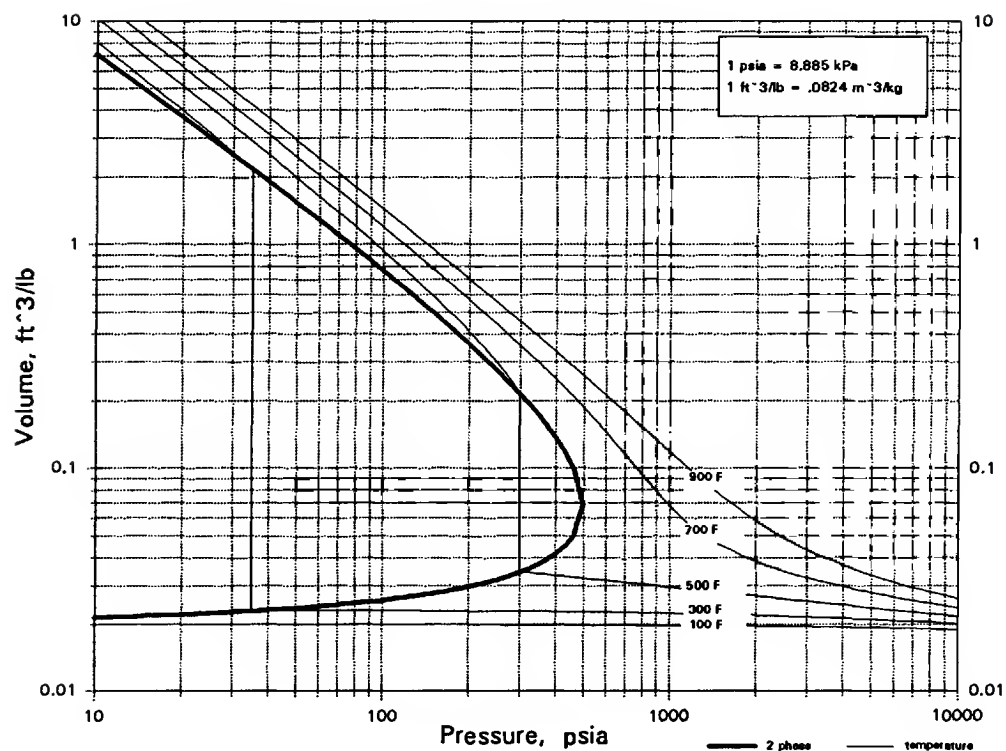
C5H9N

VALERONITRILE

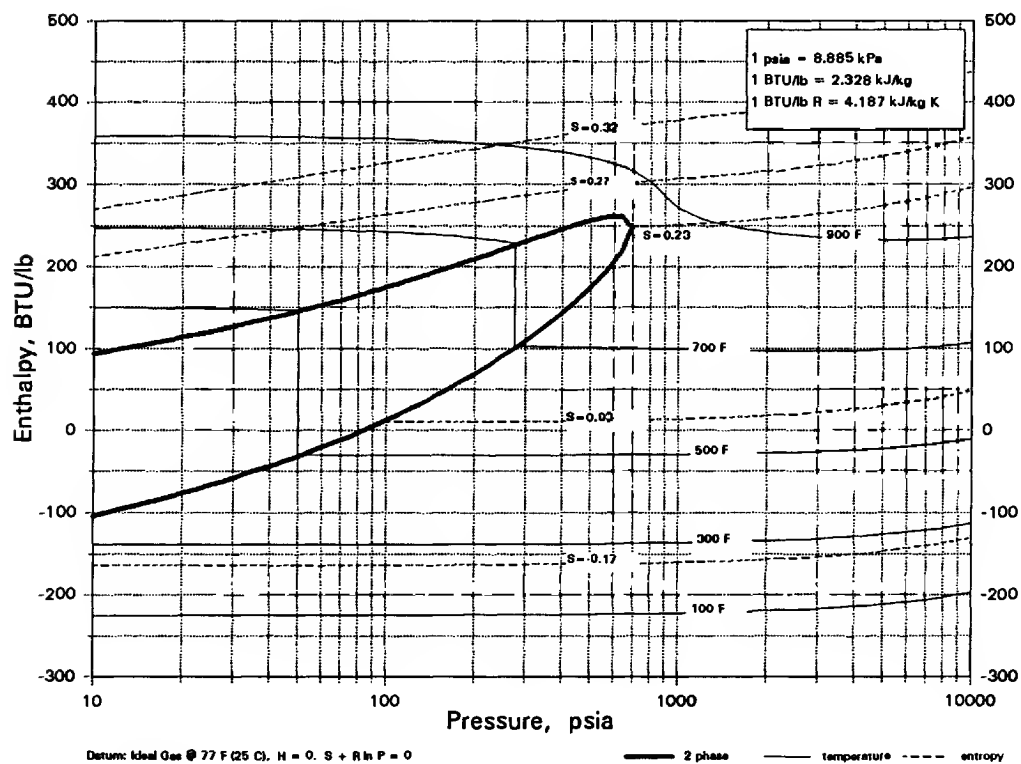
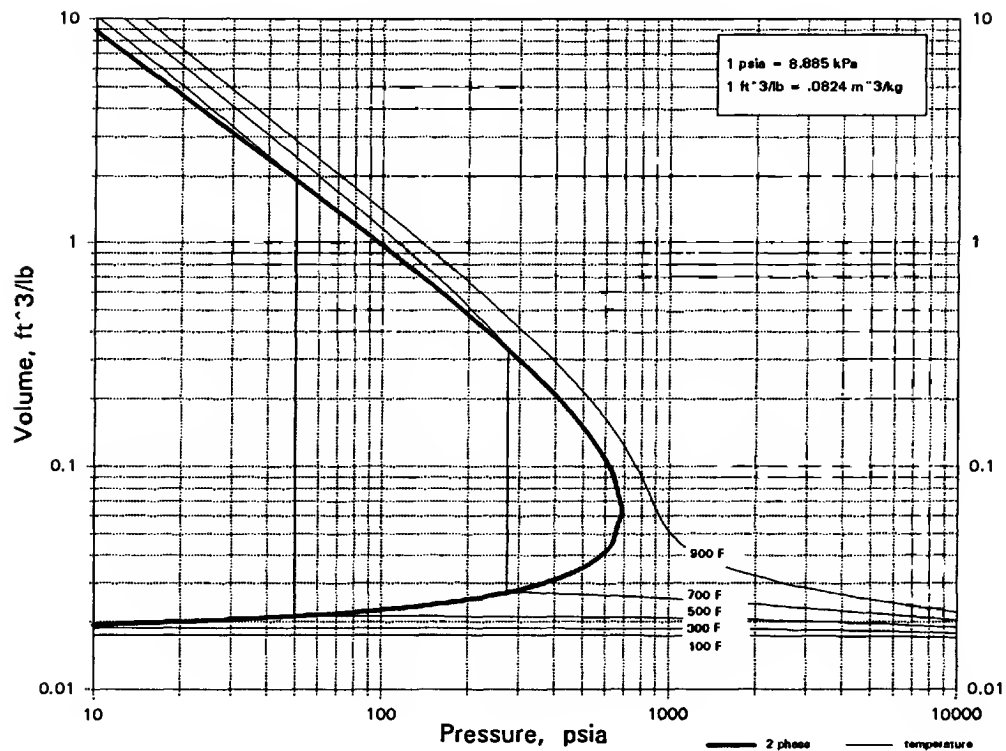


C₅H₉NO

n-BUTYL ISOCYANATE

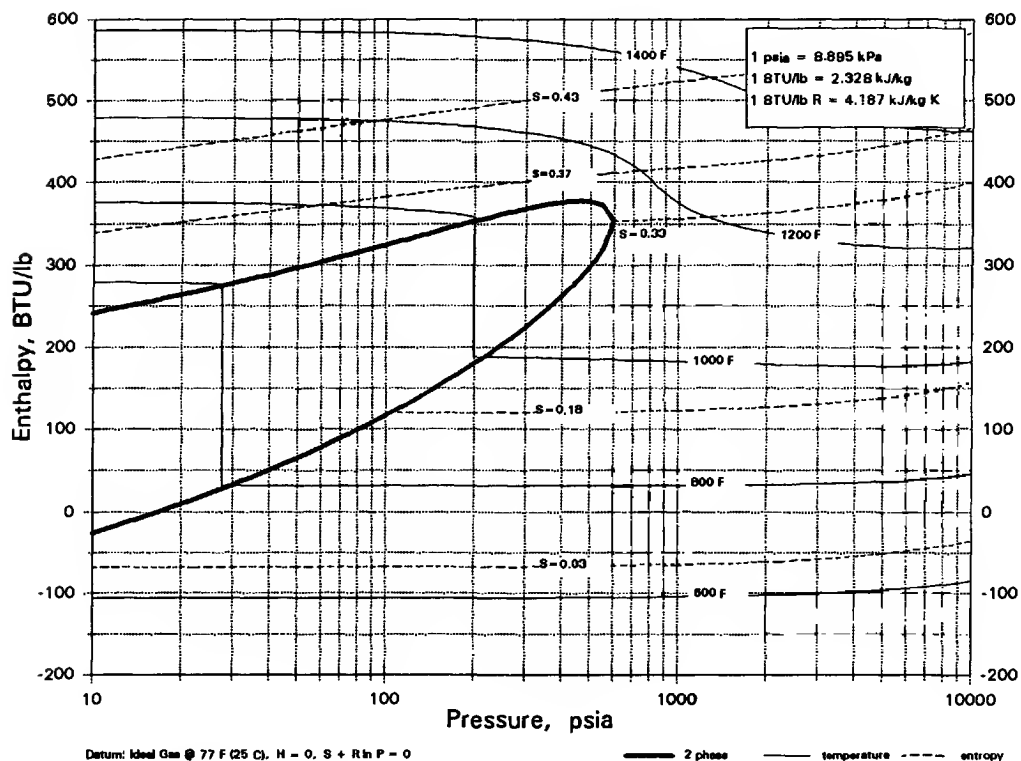
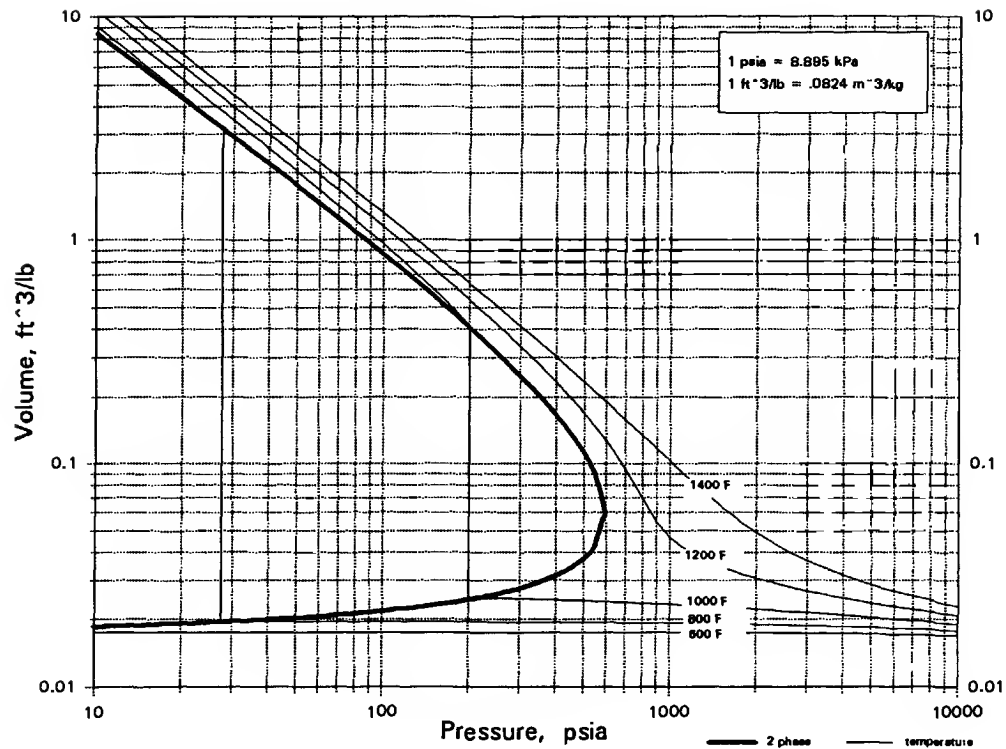


C5H9NO
N-METHYL-2-PYRROLIDONE

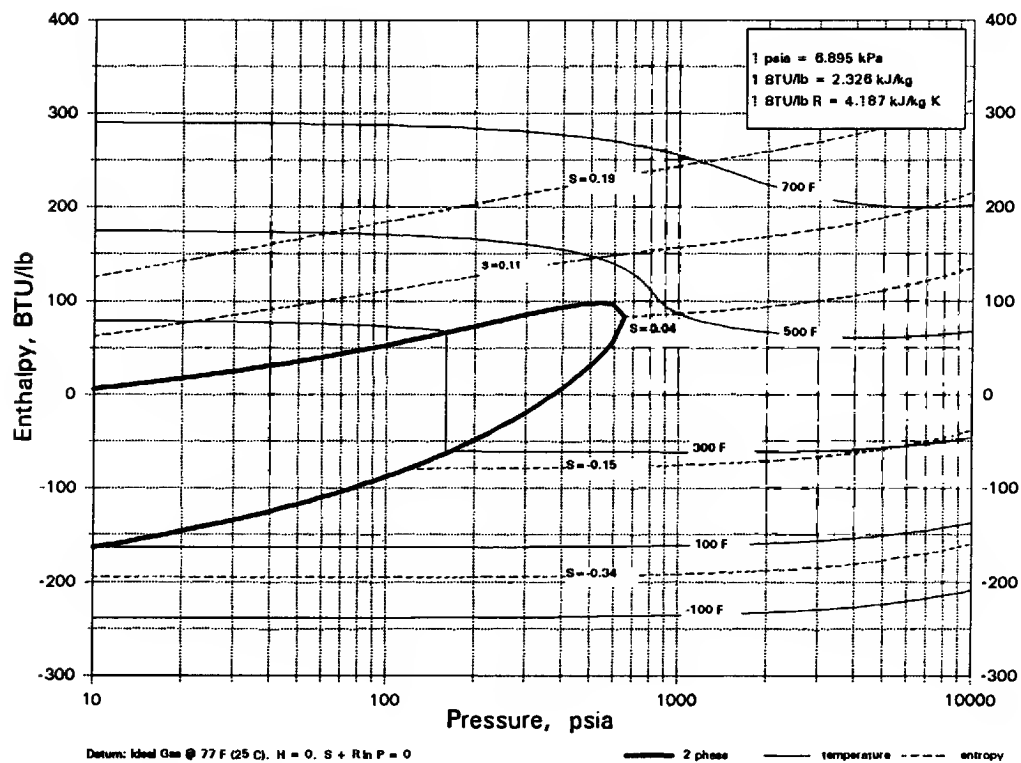
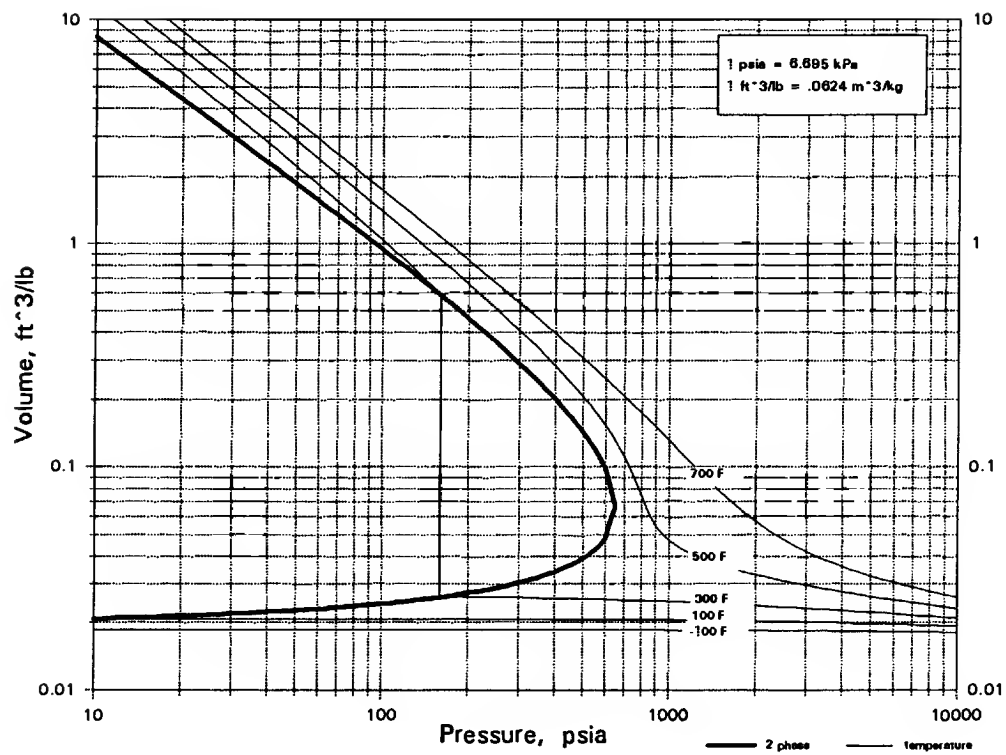


C5H9NO4

L-GLUTAMIC ACID

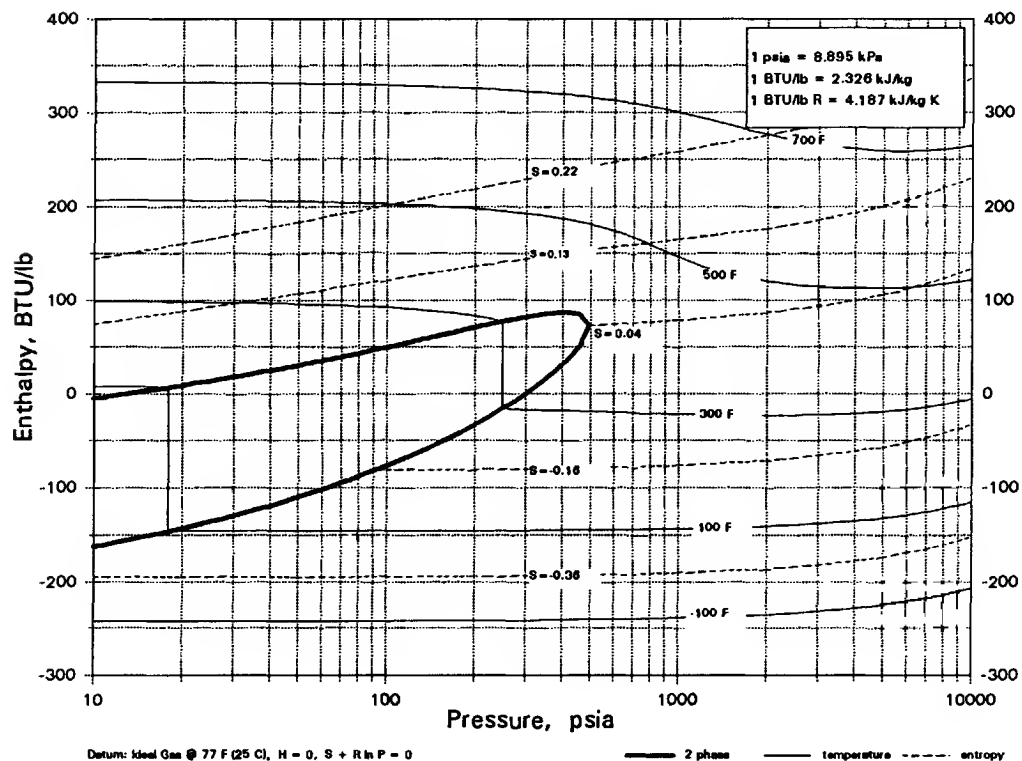
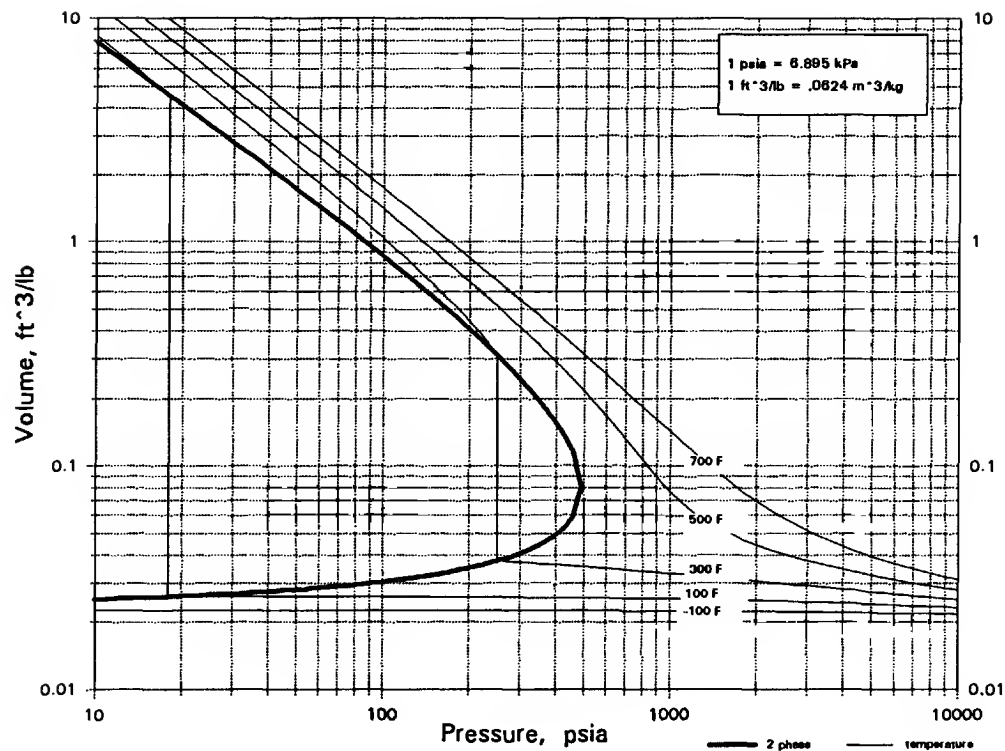


C5H10
CYCLOPENTANE



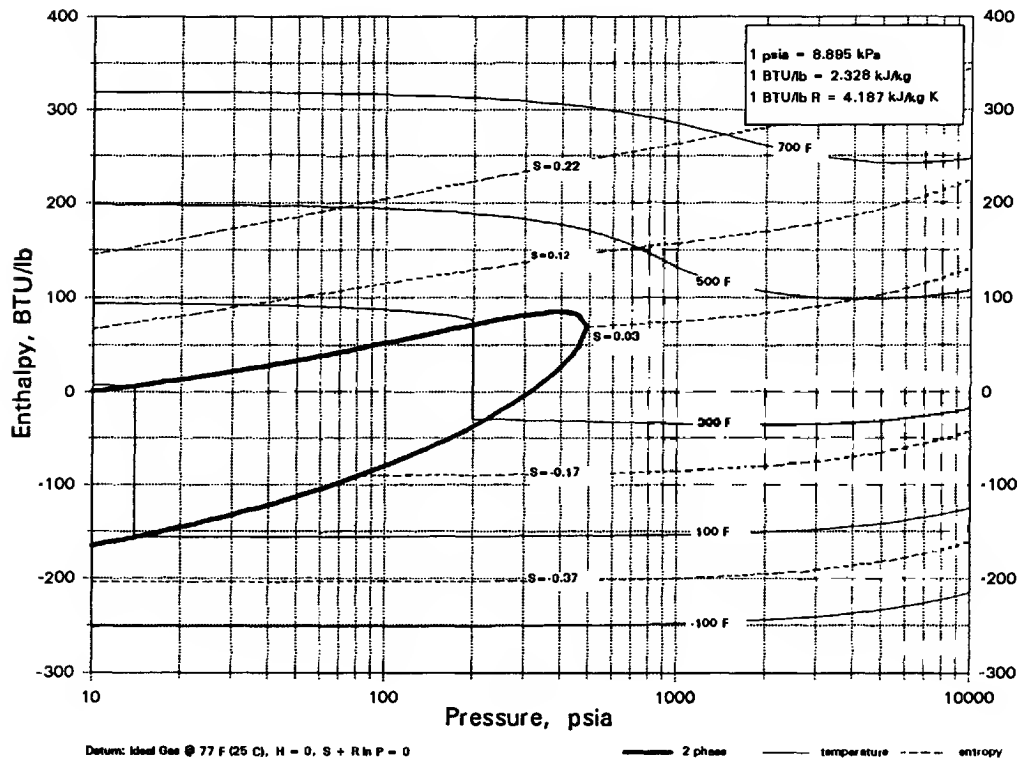
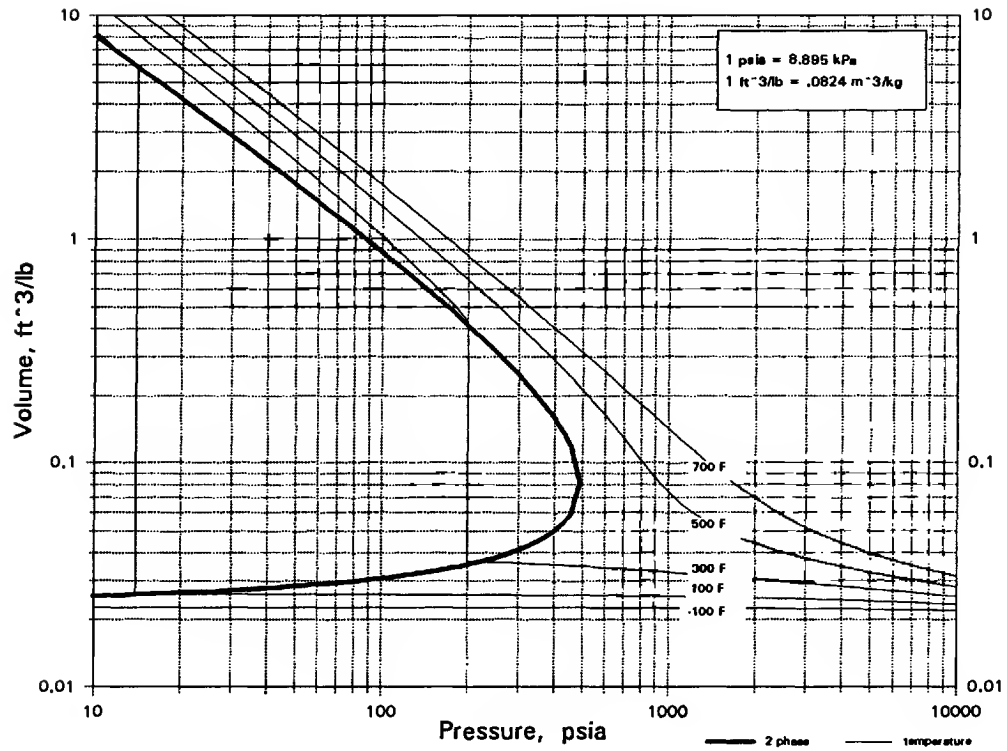
C5H10

2-METHYL-1-BUTENE



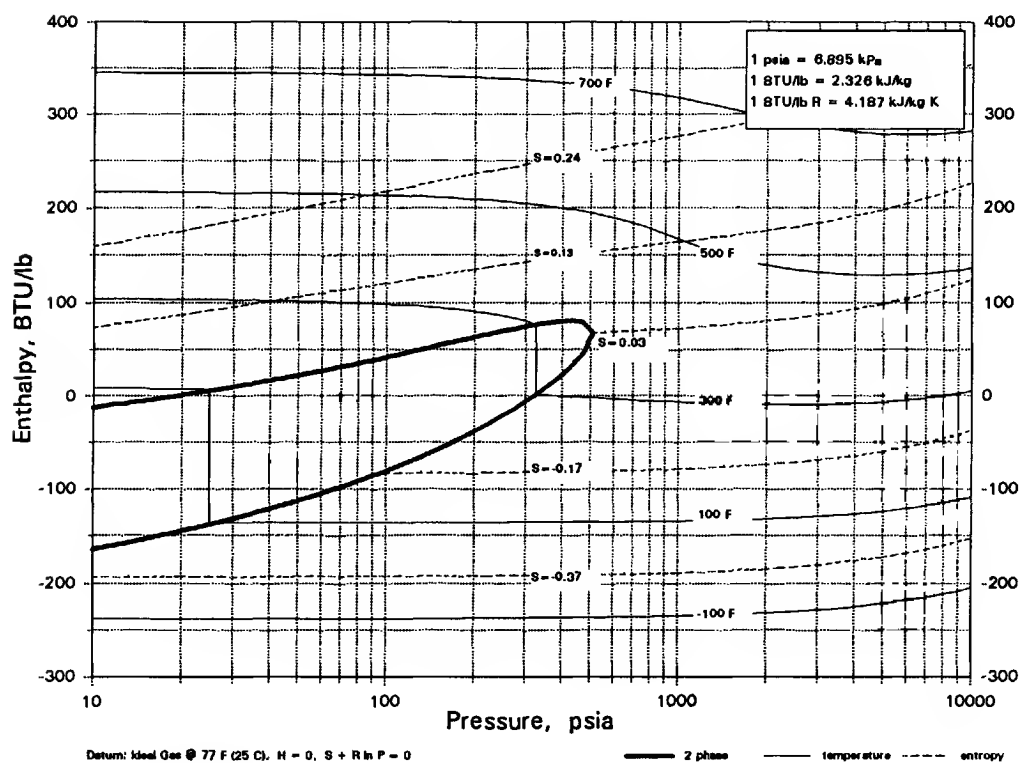
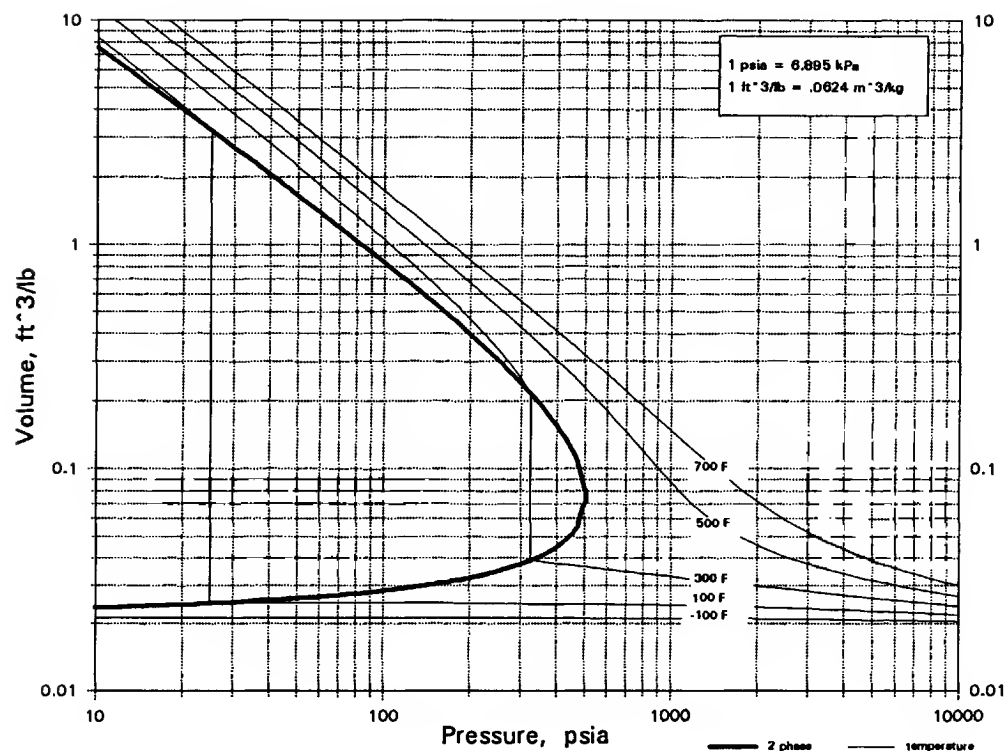
C5H10

2-METHYL-2-BUTENE



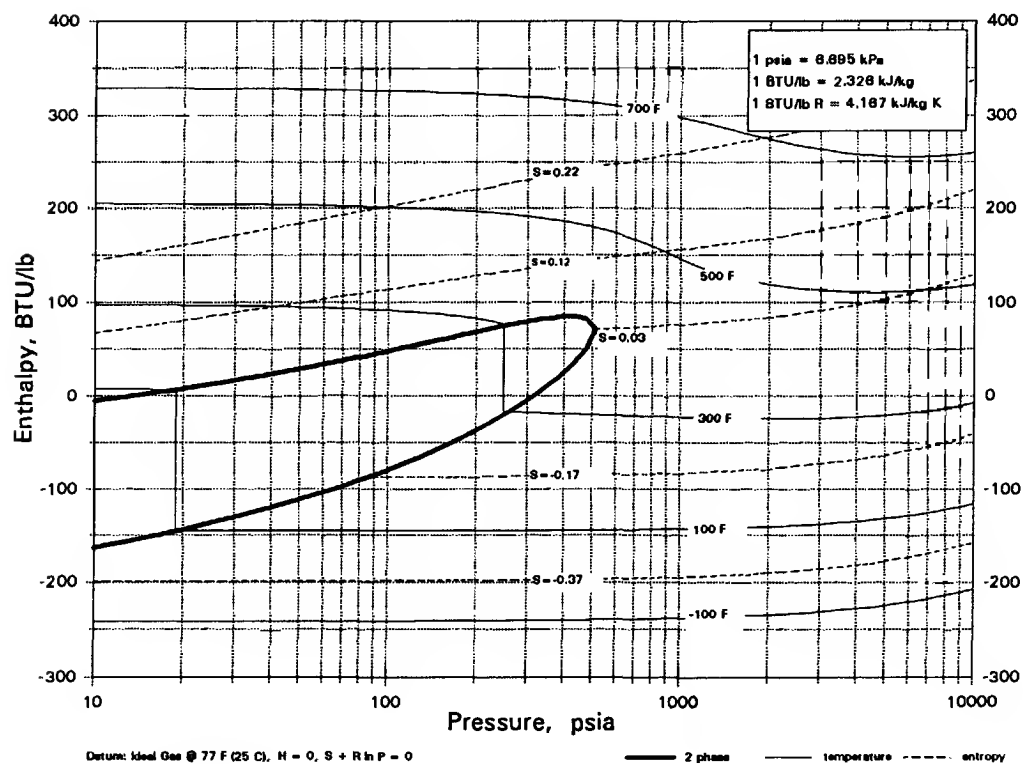
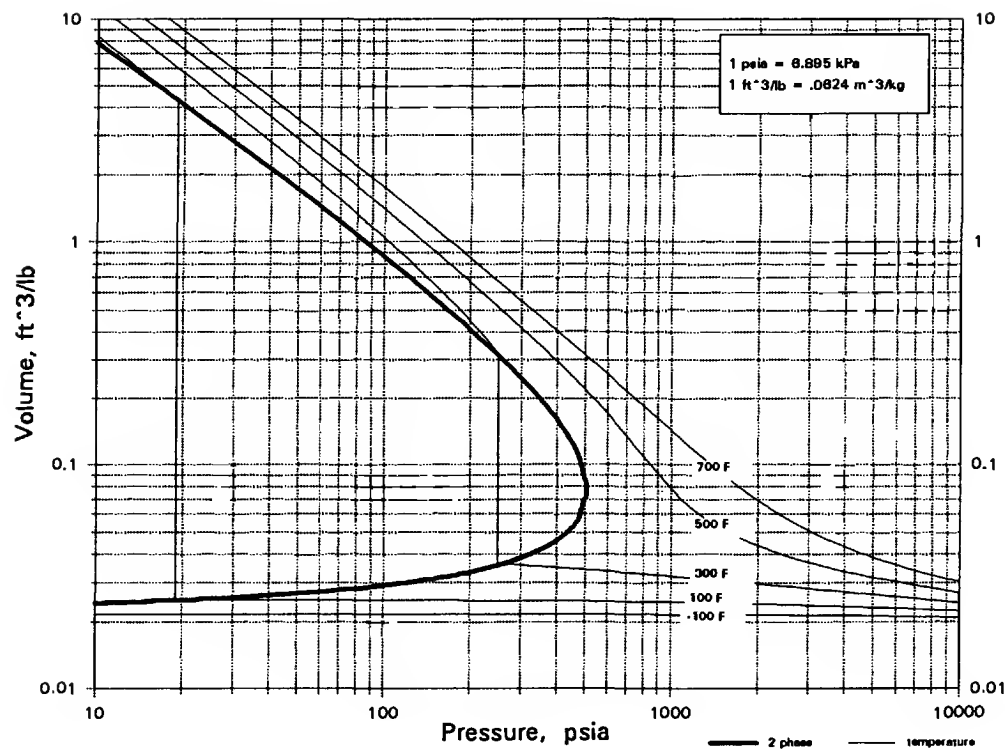
C5H10

3-METHYL-1-BUTENE



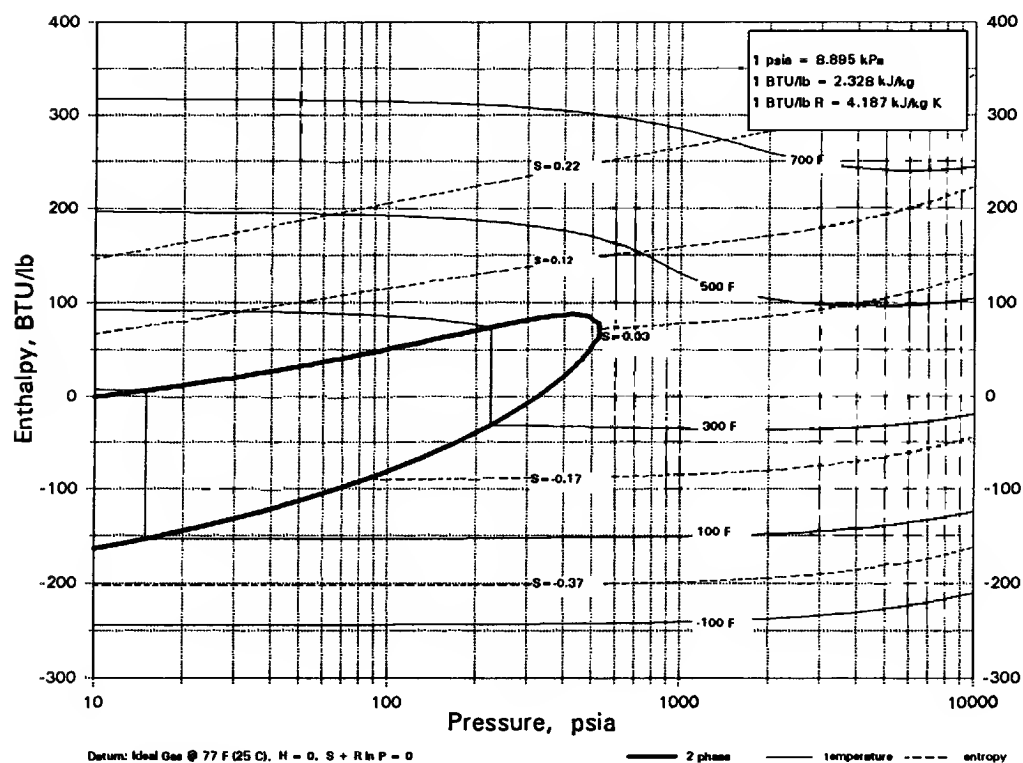
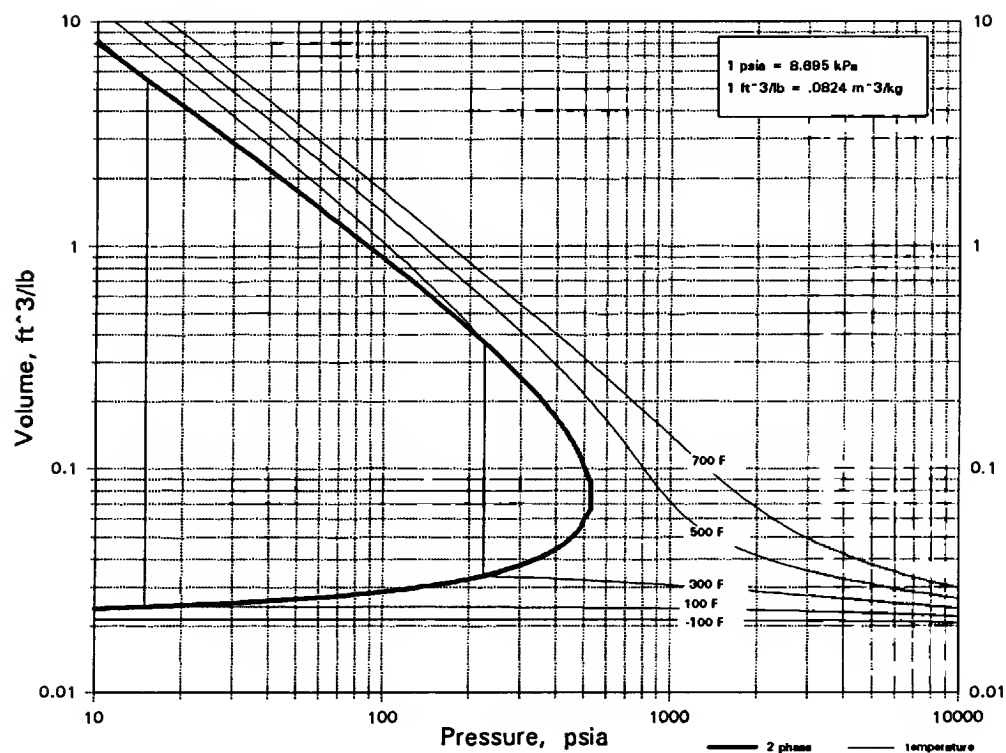
C5H10

1-PENTENE



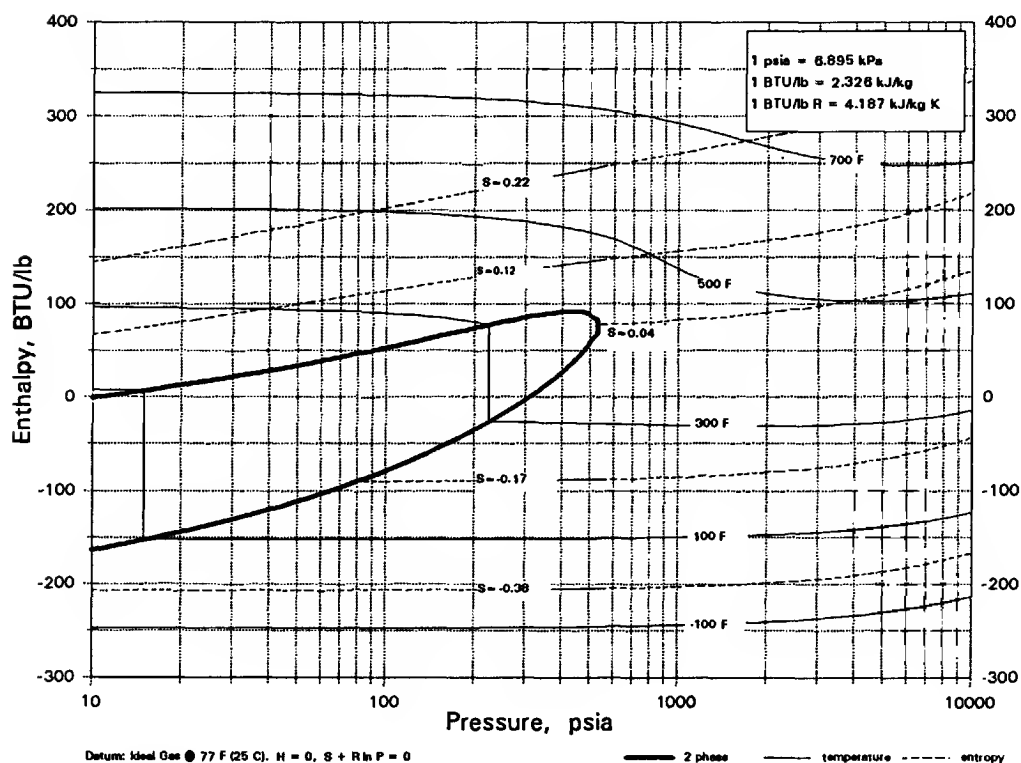
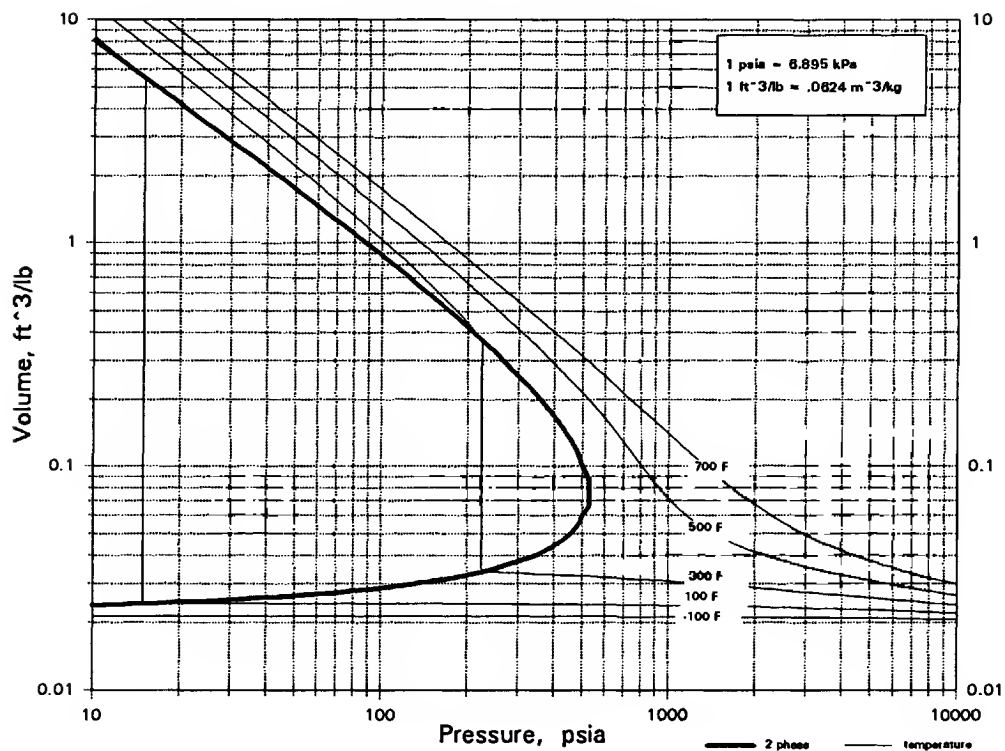
C5H10

cis-2-PENTENE

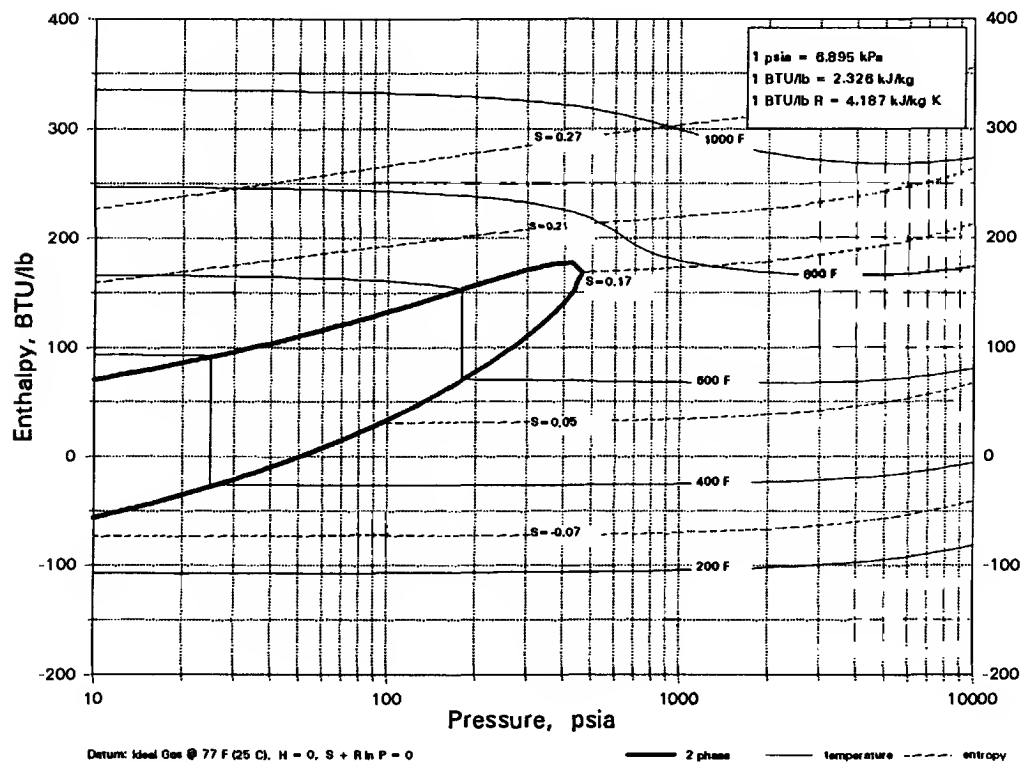
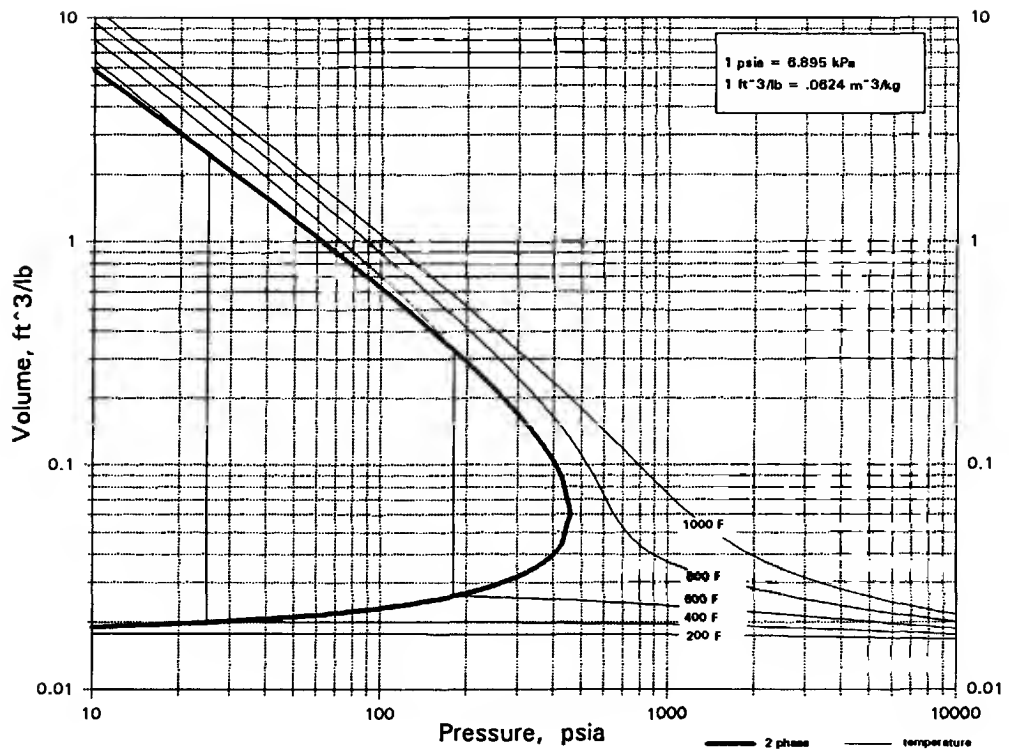


C5H10

trans-2-PENTENE

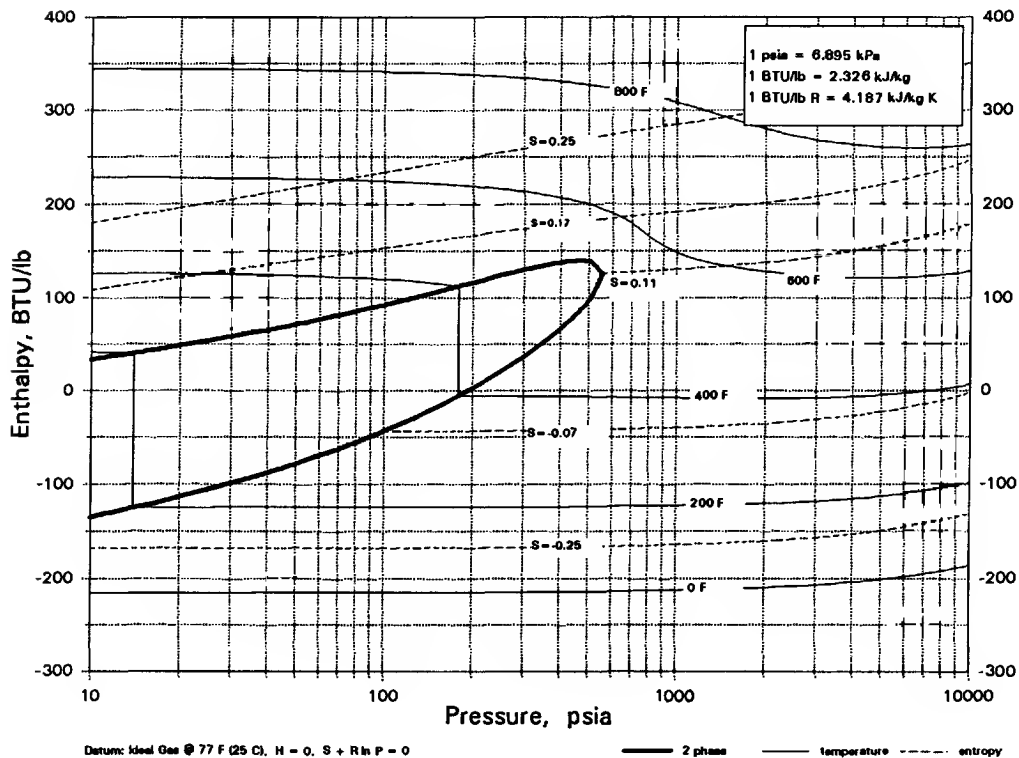
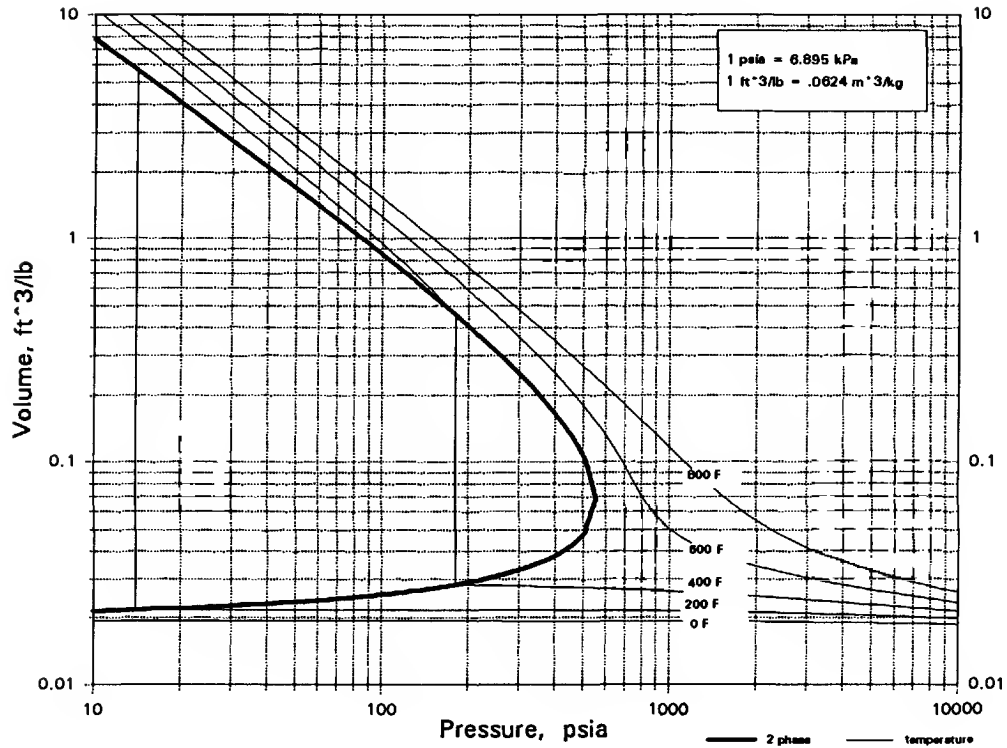


C5H10Cl2
1-5-DICHLOROPENTANE



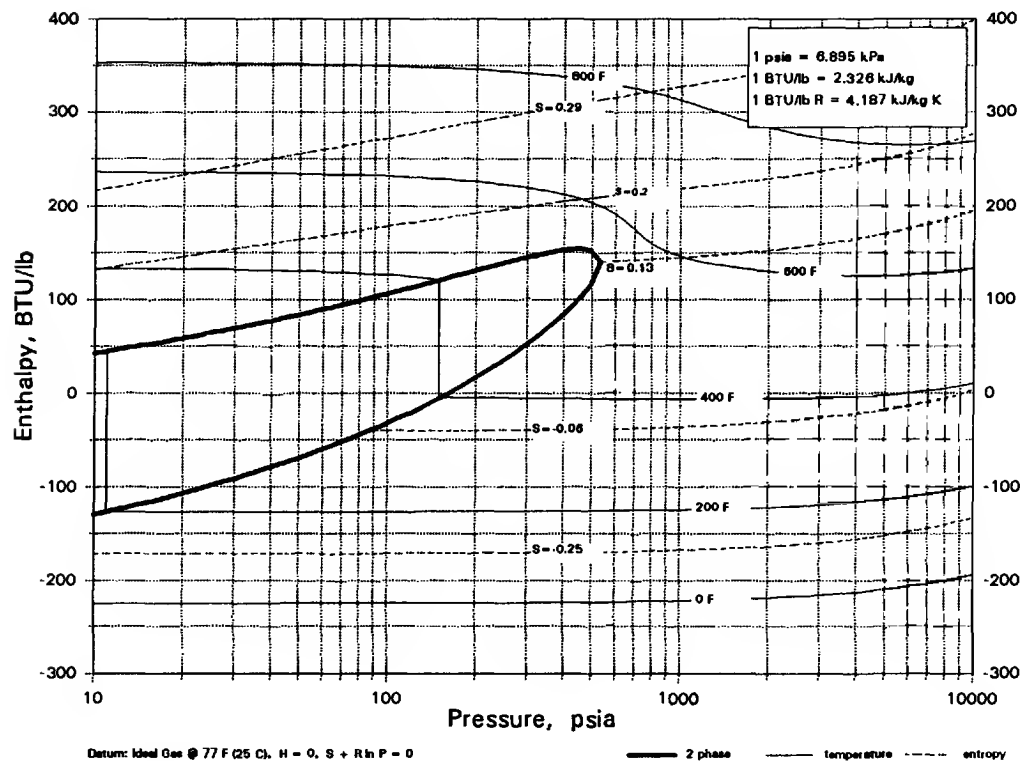
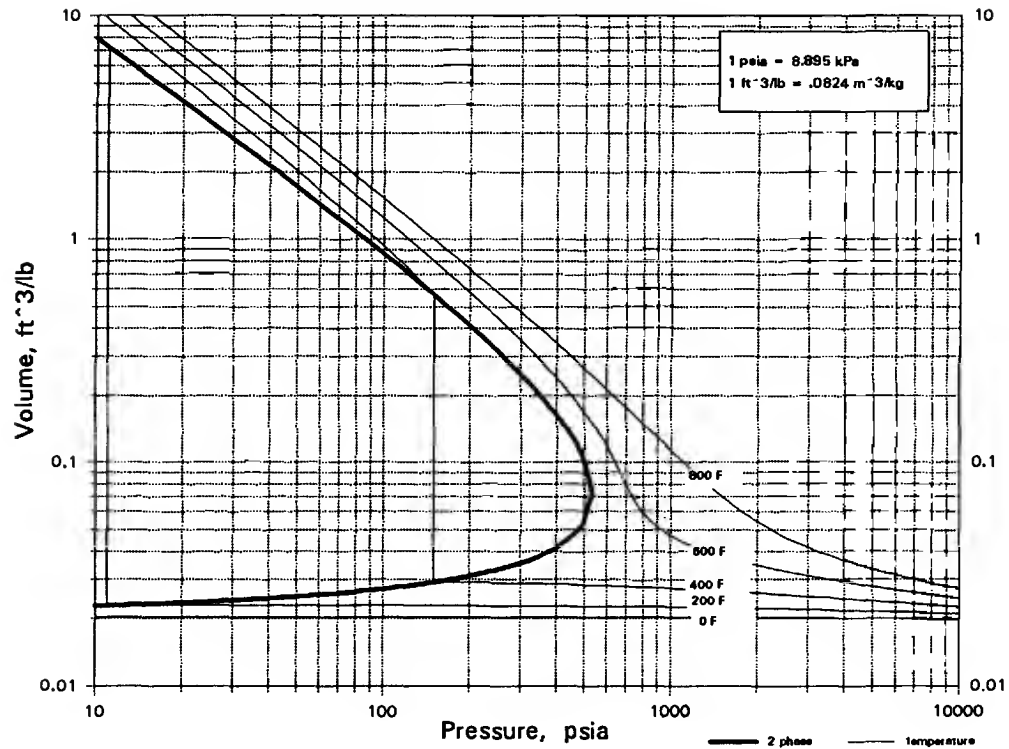
C5H10O

METHYL ISOPROPYL KETONE



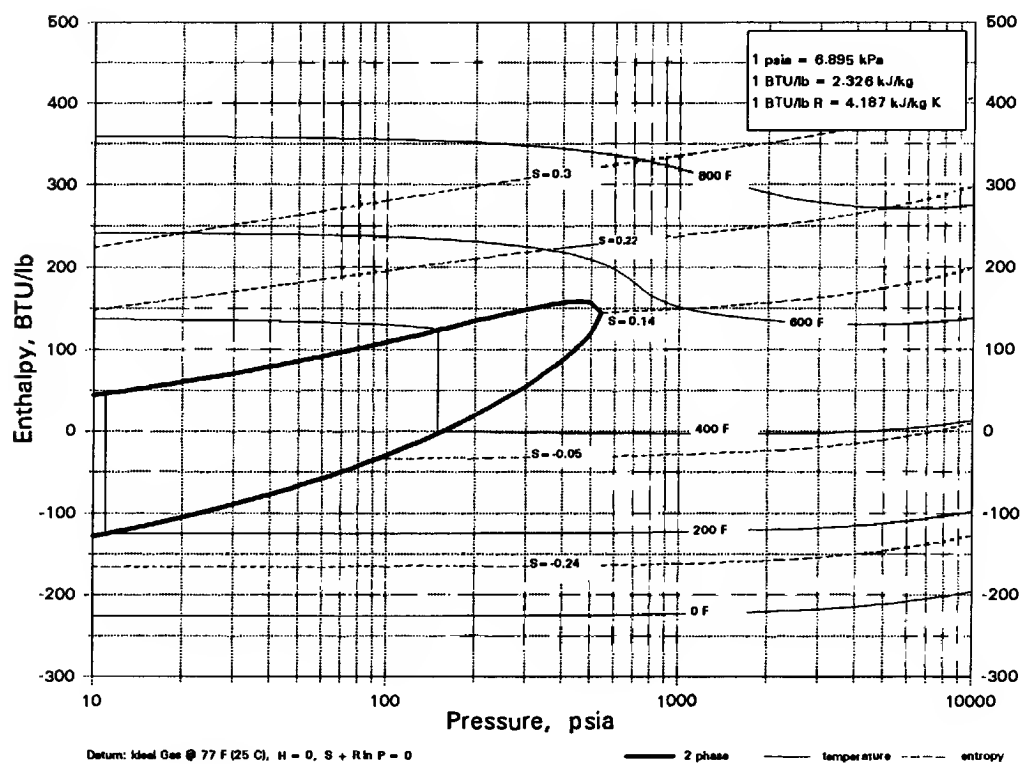
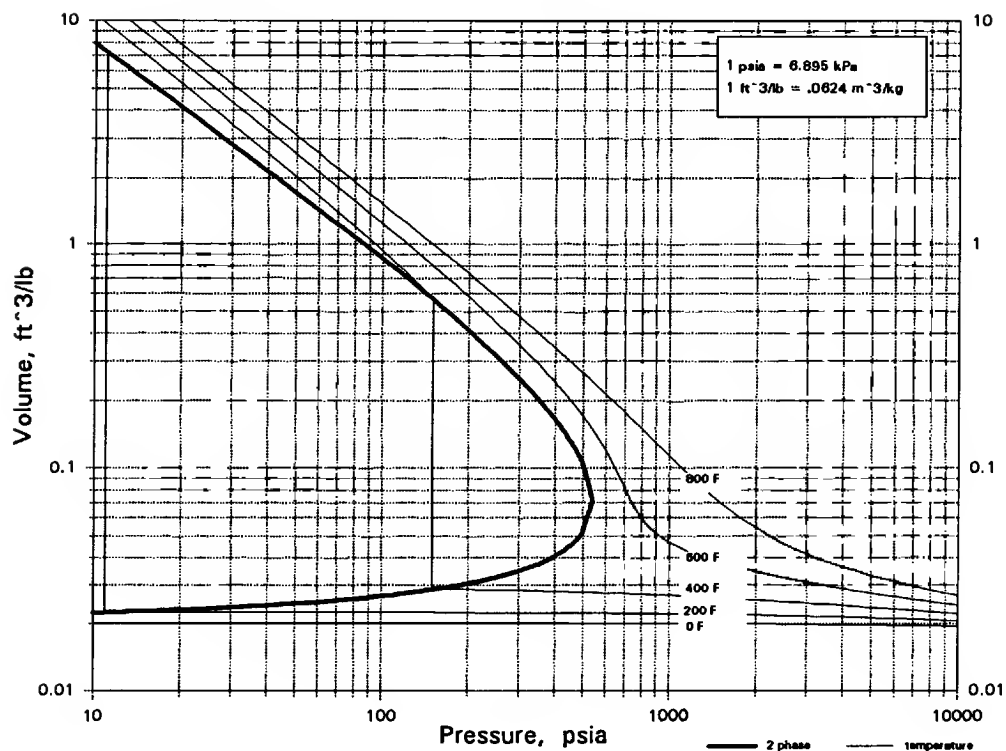
C5H10O

2-PENTANONE

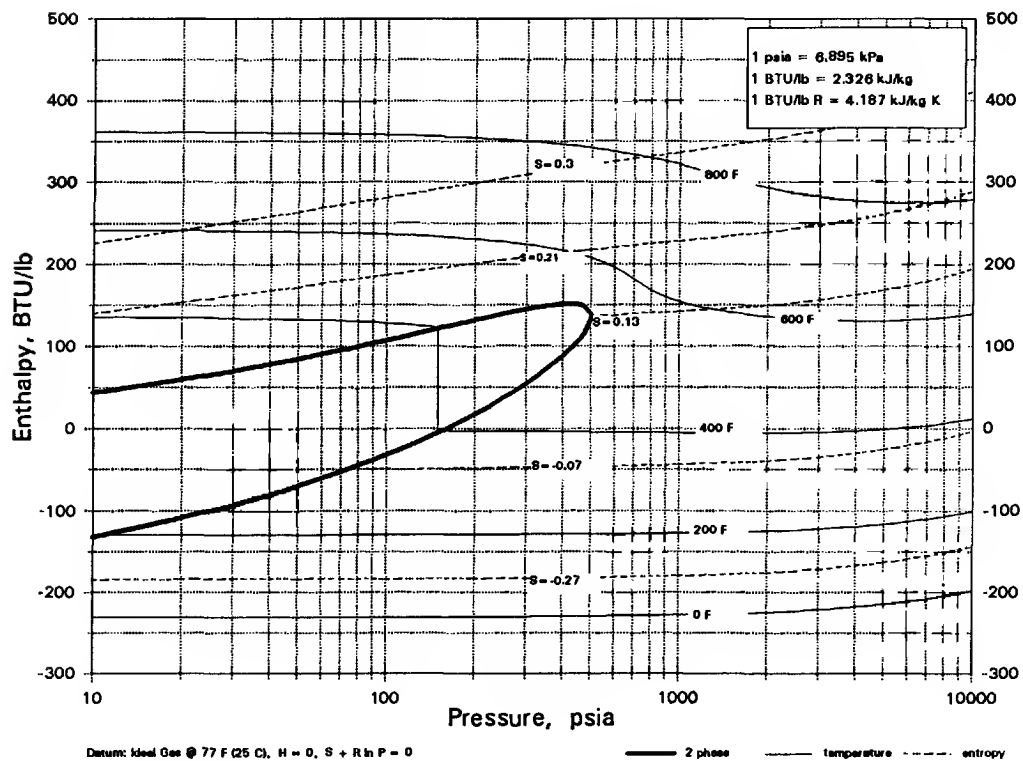
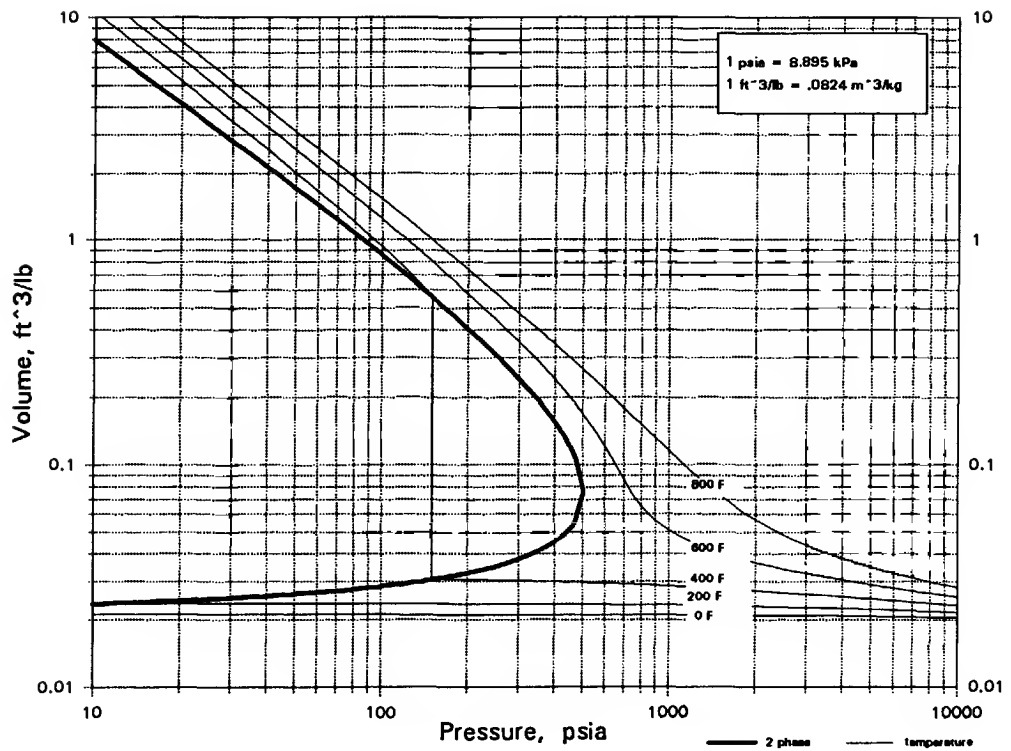


C5H10O

DIETHYL KETONE

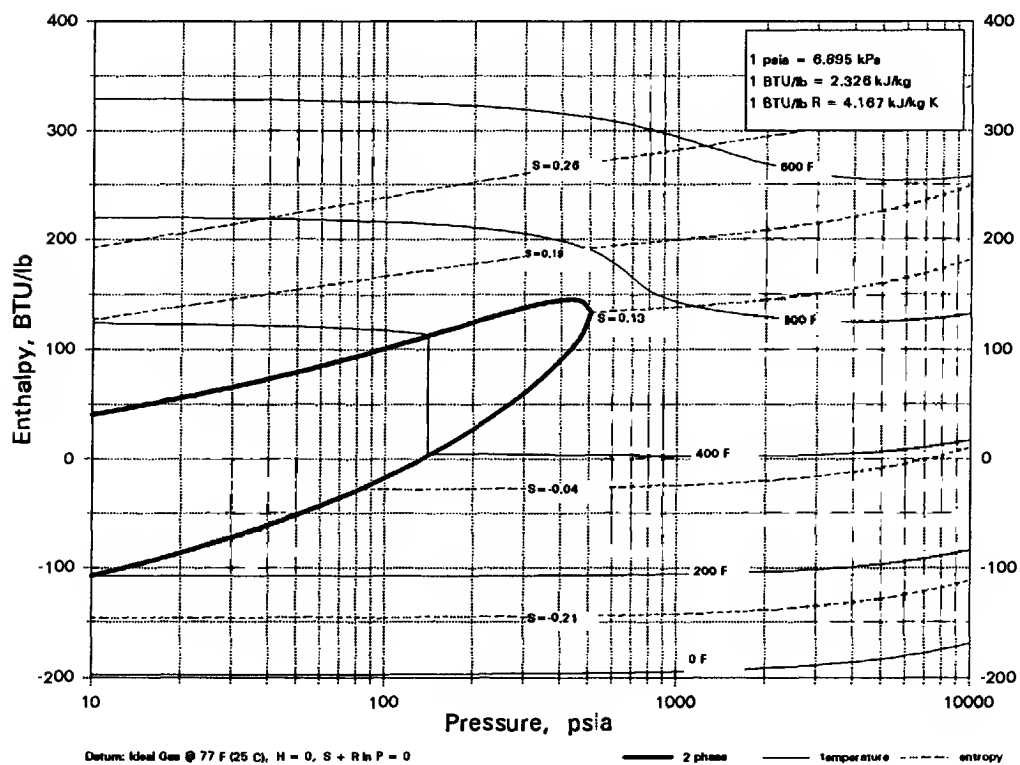
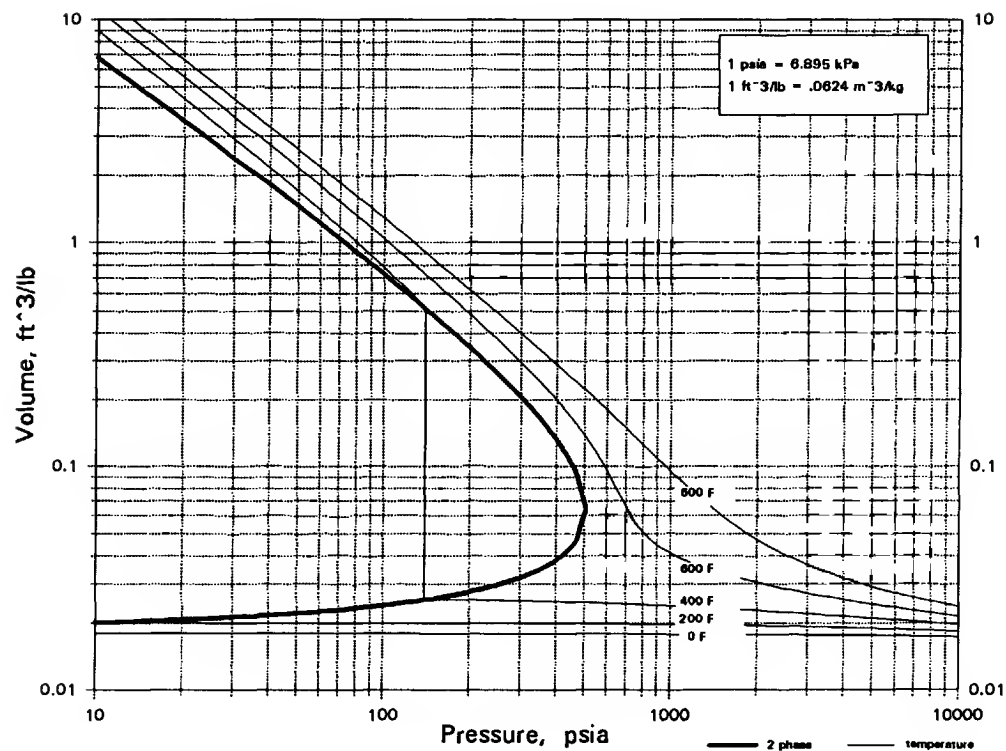


C5H10O
VALERALDEHYDE



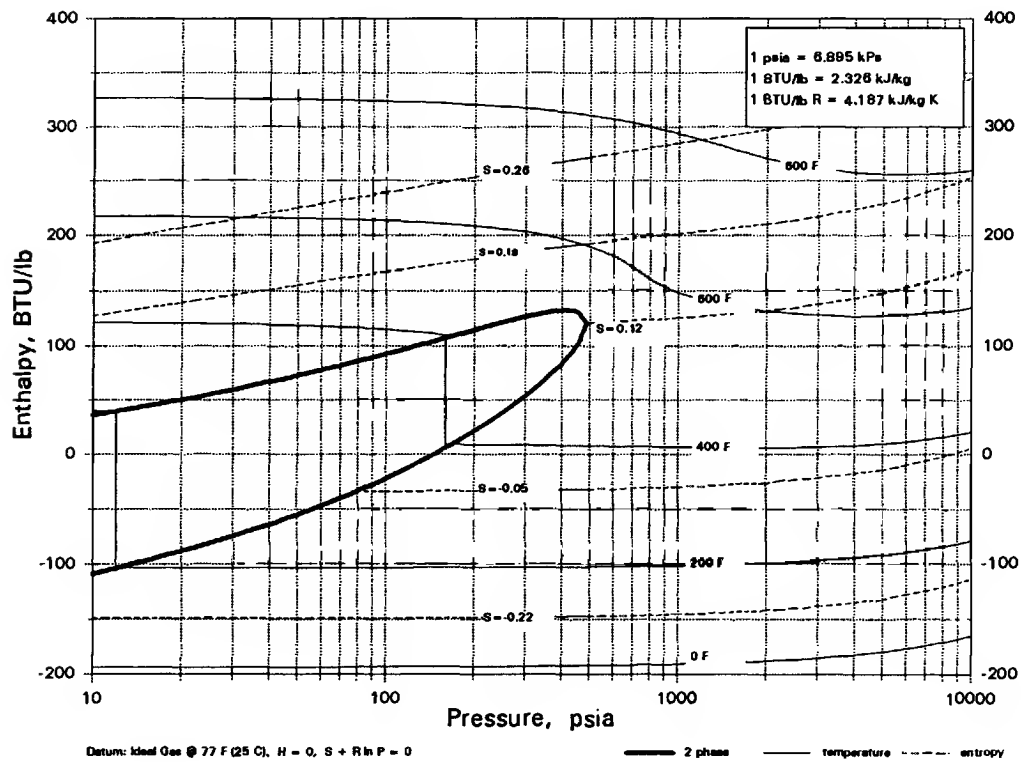
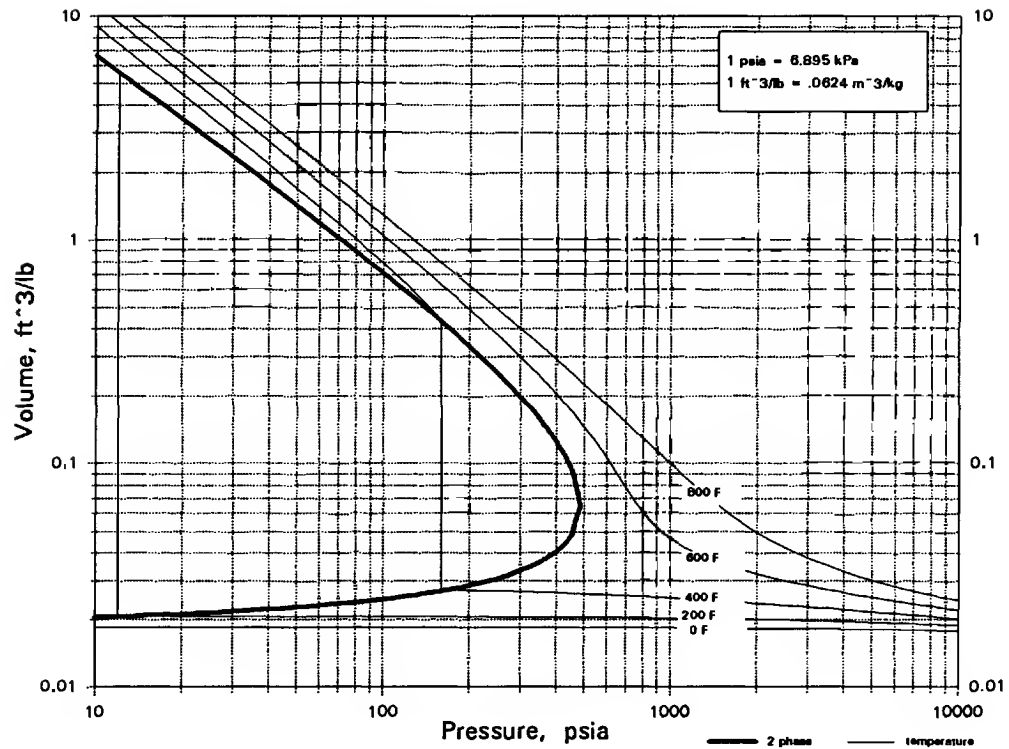
C5H10O2

n-BUTYL FORMATE



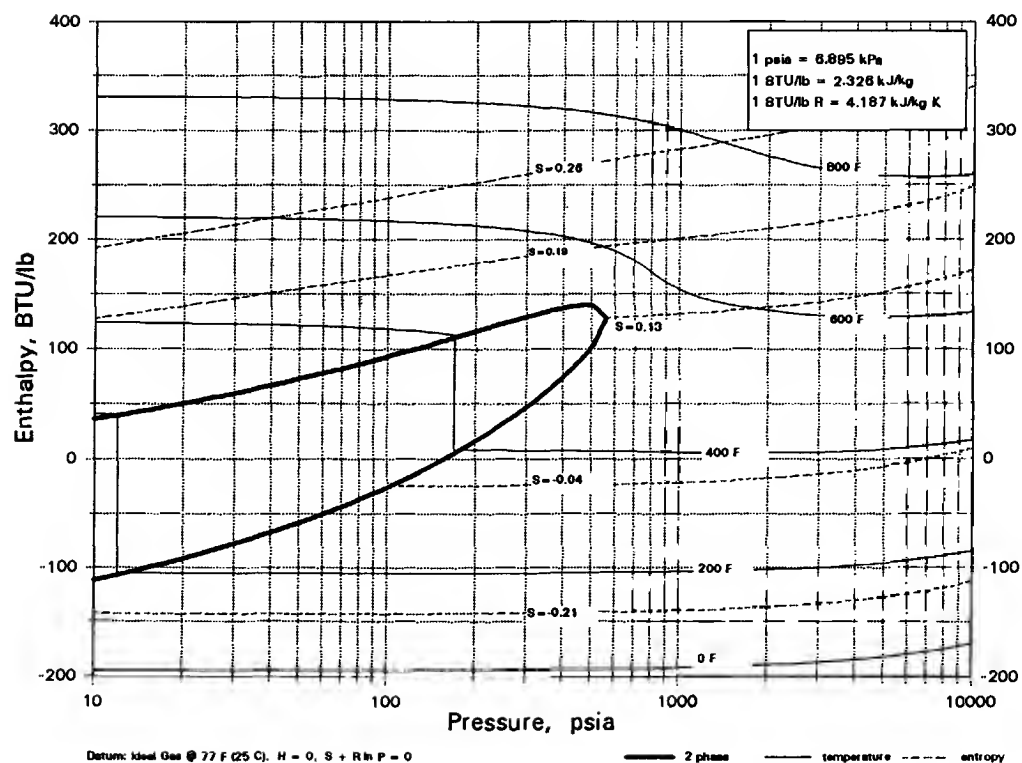
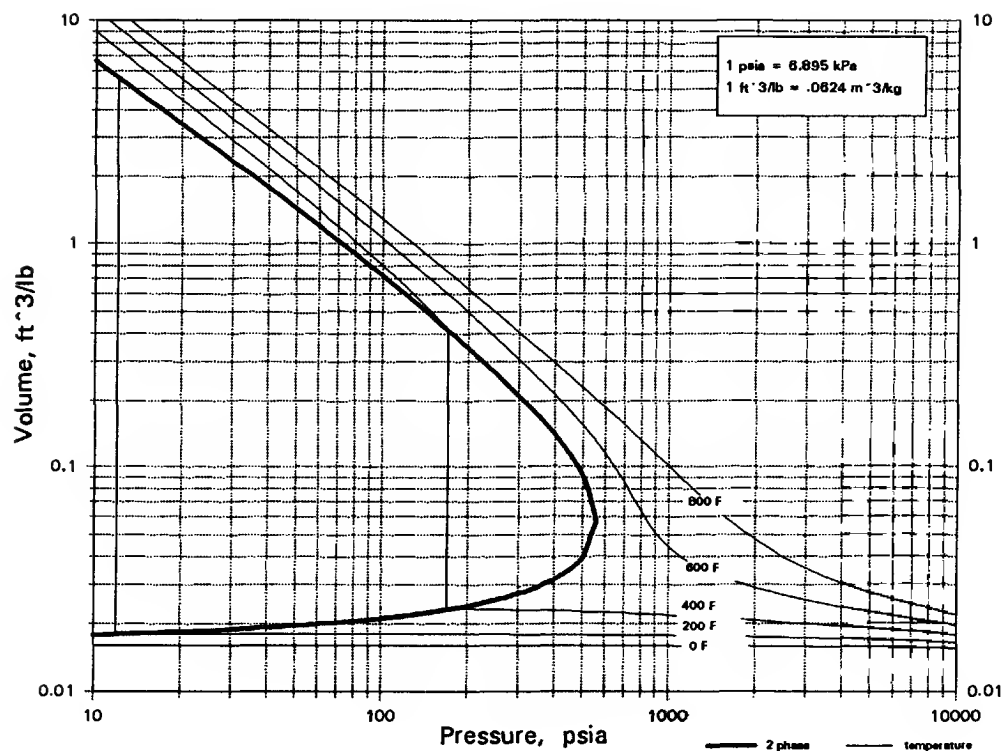
C5H10O2

ETHYL PROPIONATE



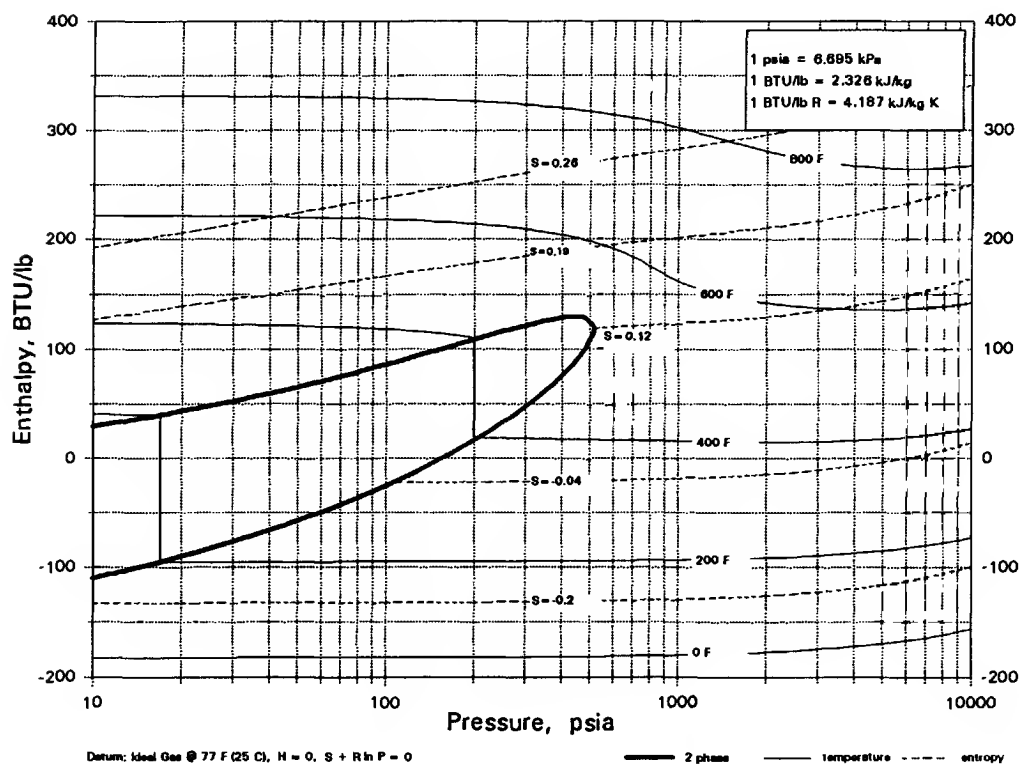
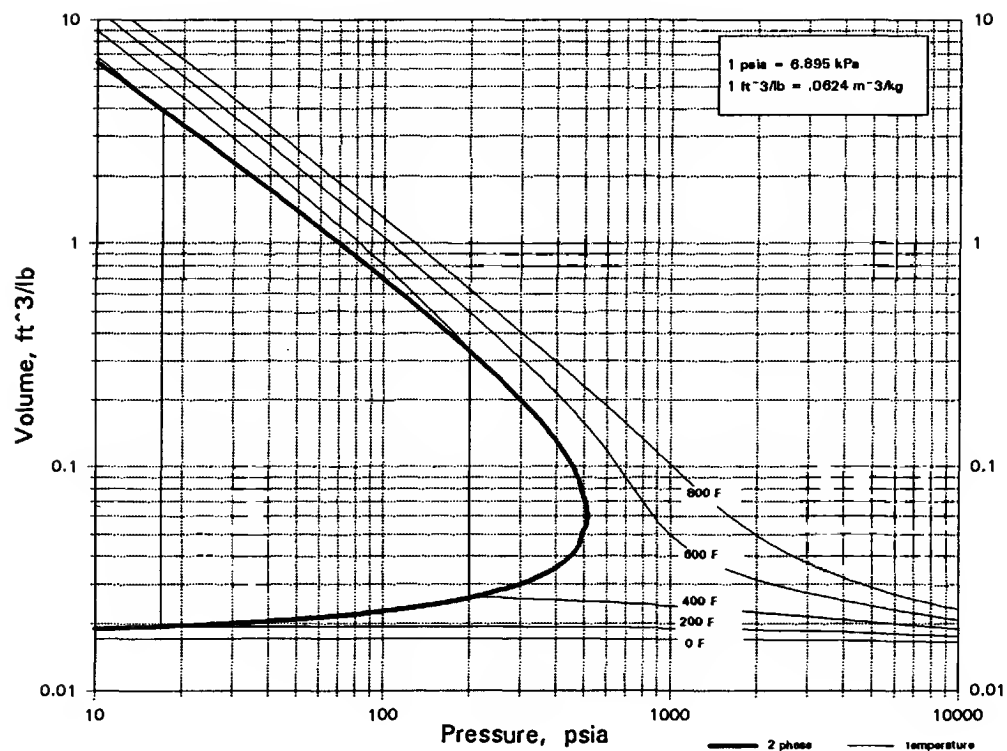
C5H10O2

ISOBUTYL FORMATE



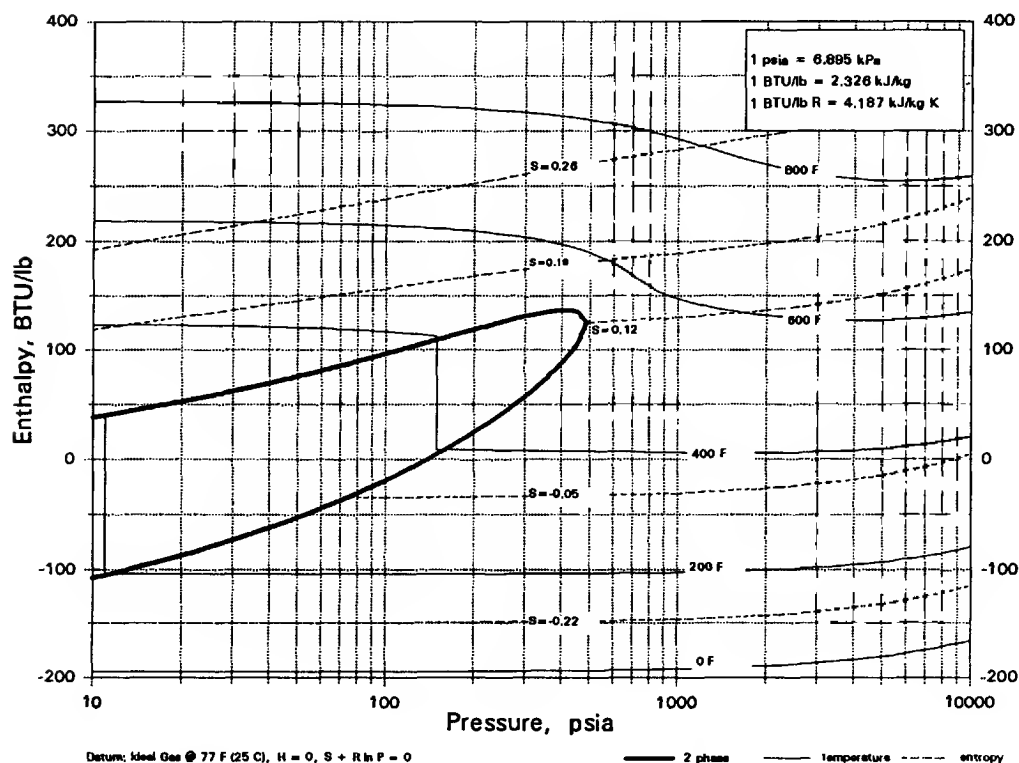
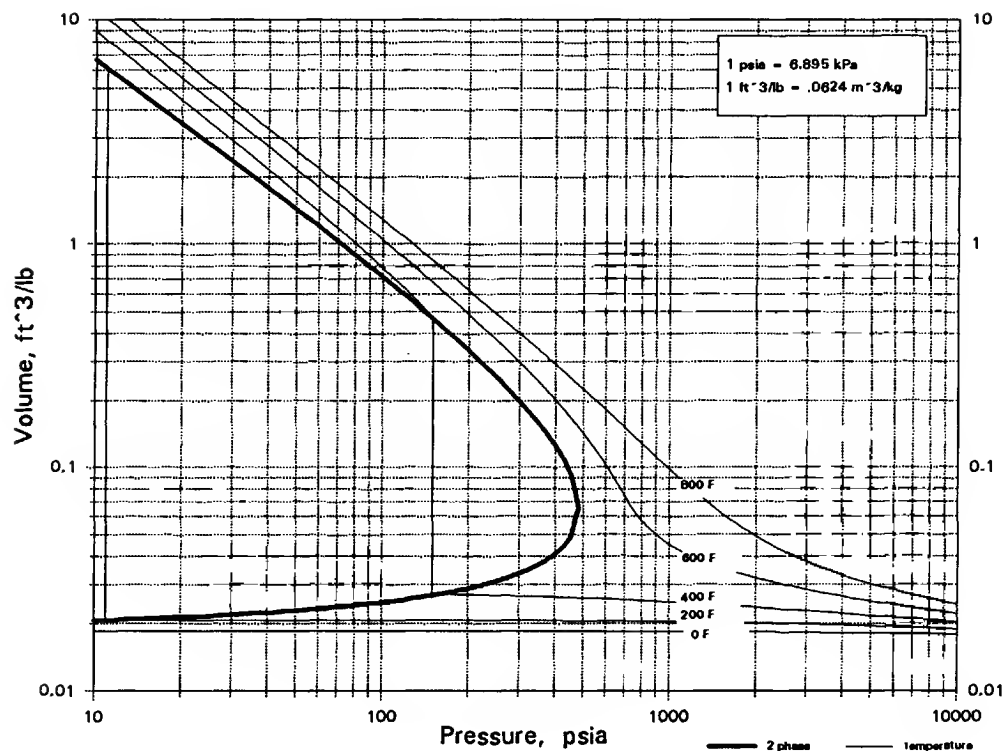
C5H10O2

ISOPROPYL ACETATE



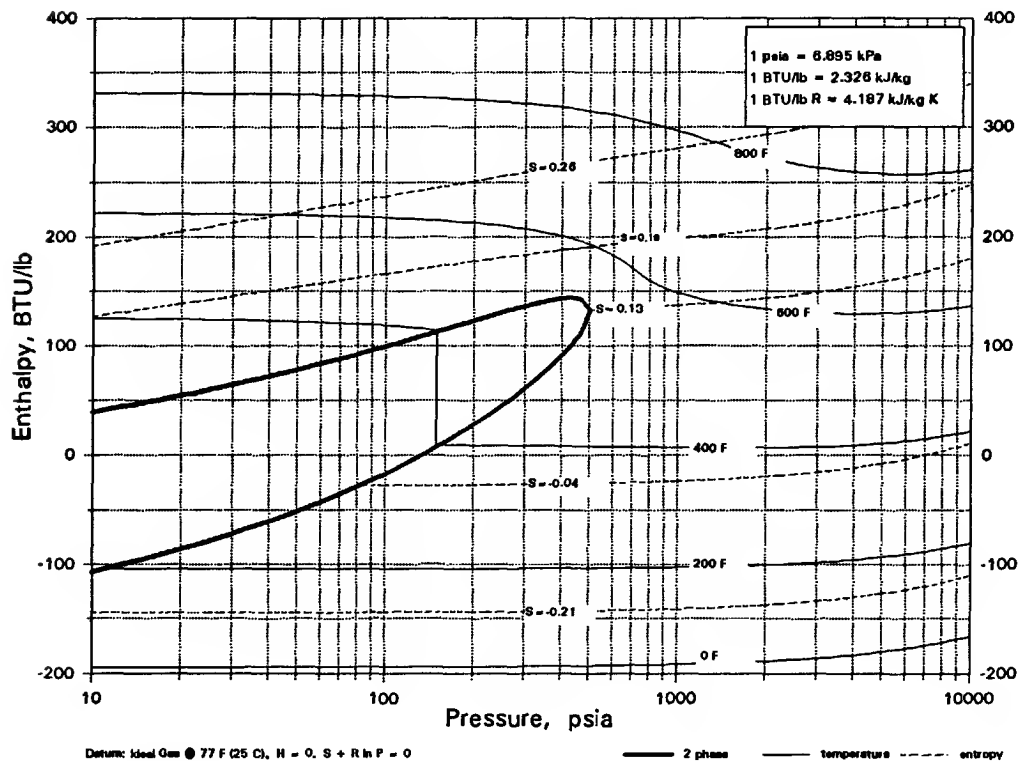
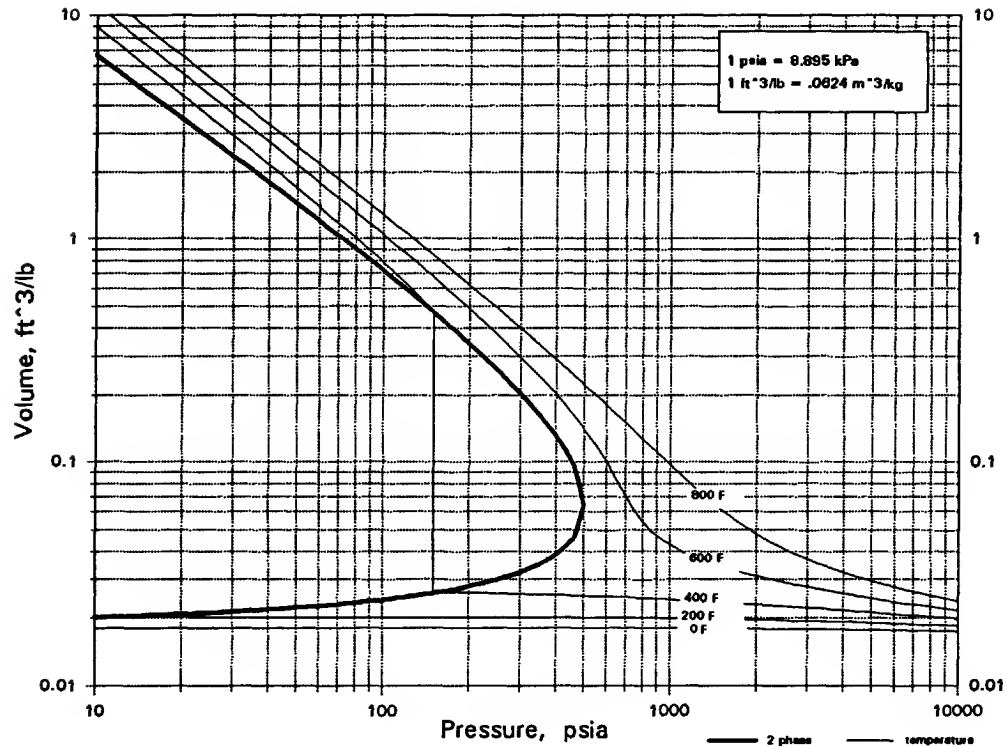
C5H10O2

n-PROPYL ACETATE



C5H10O2

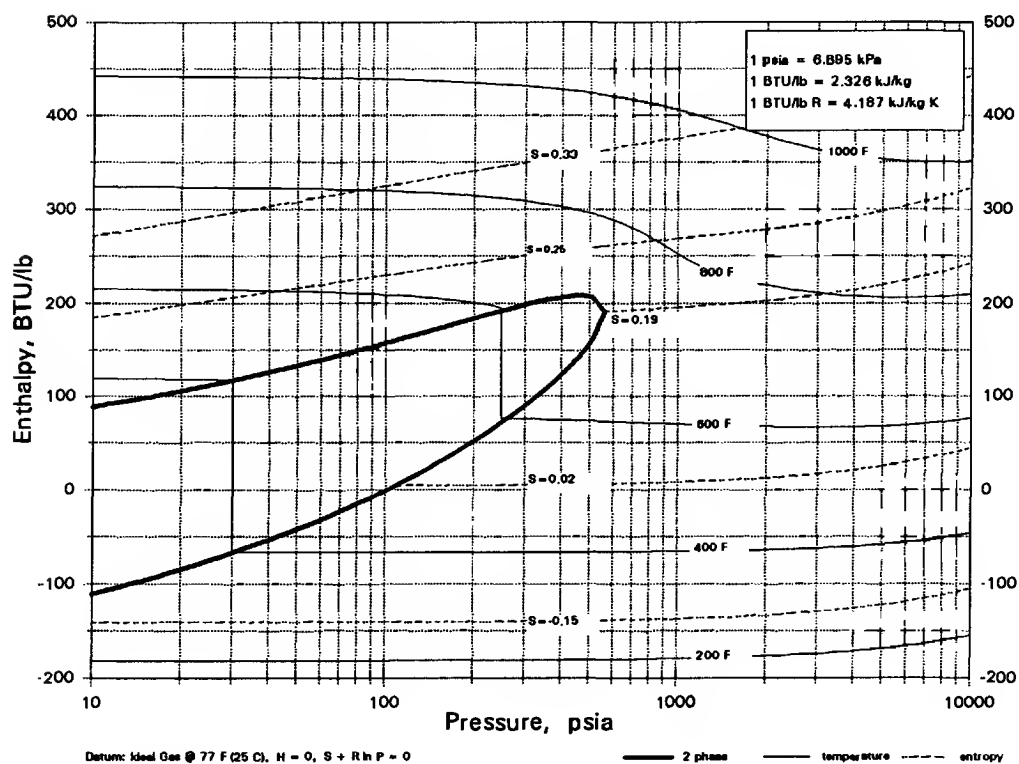
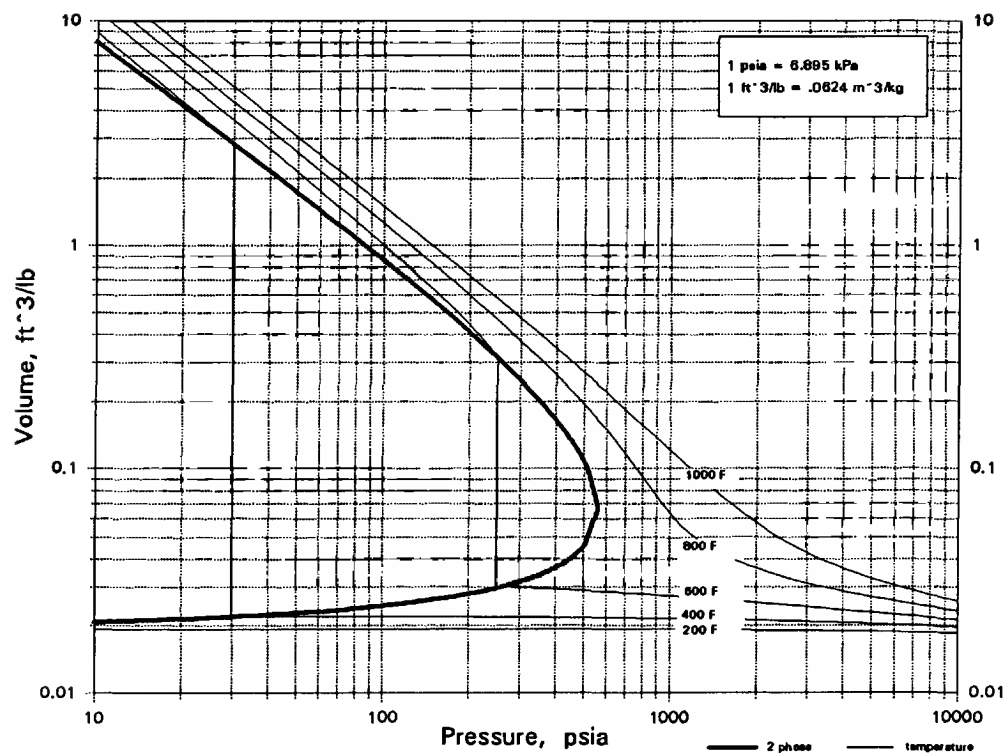
METHYL n-BUTYRATE



Detum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

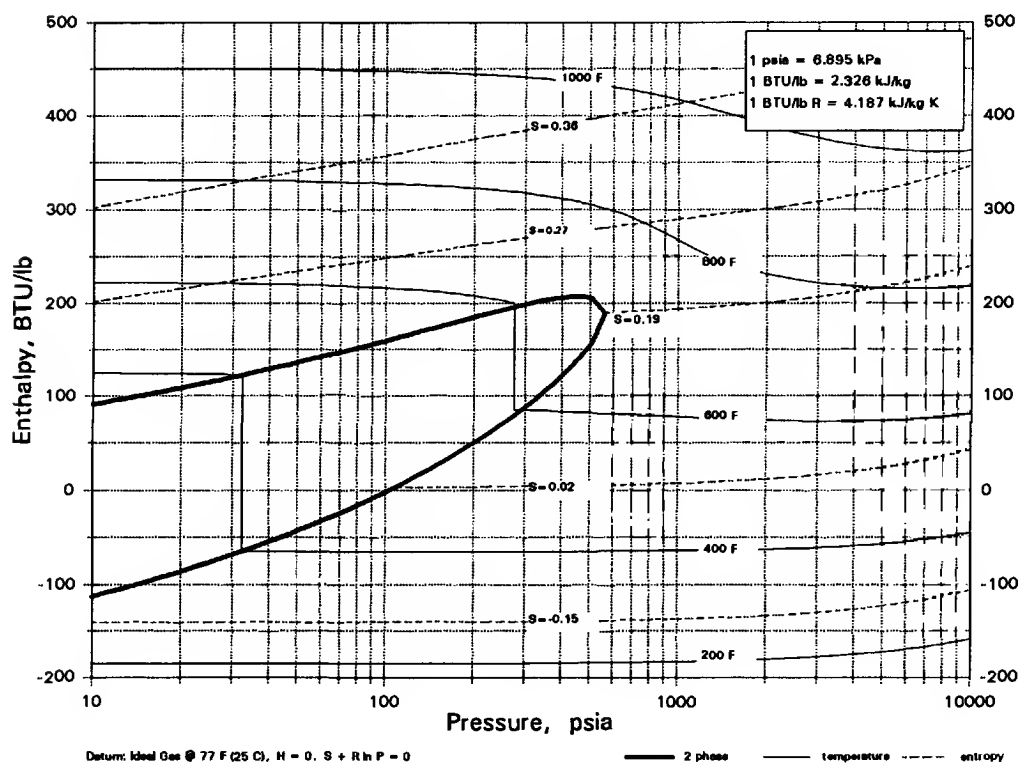
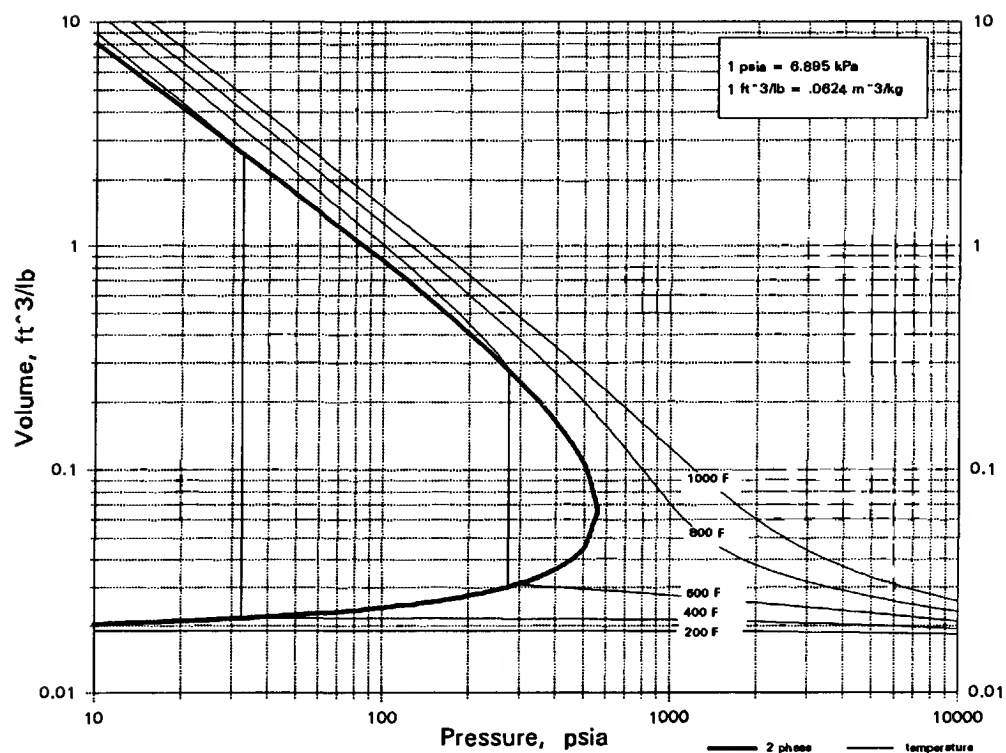
C5H10O2

2-METHYLBUTYRIC ACID



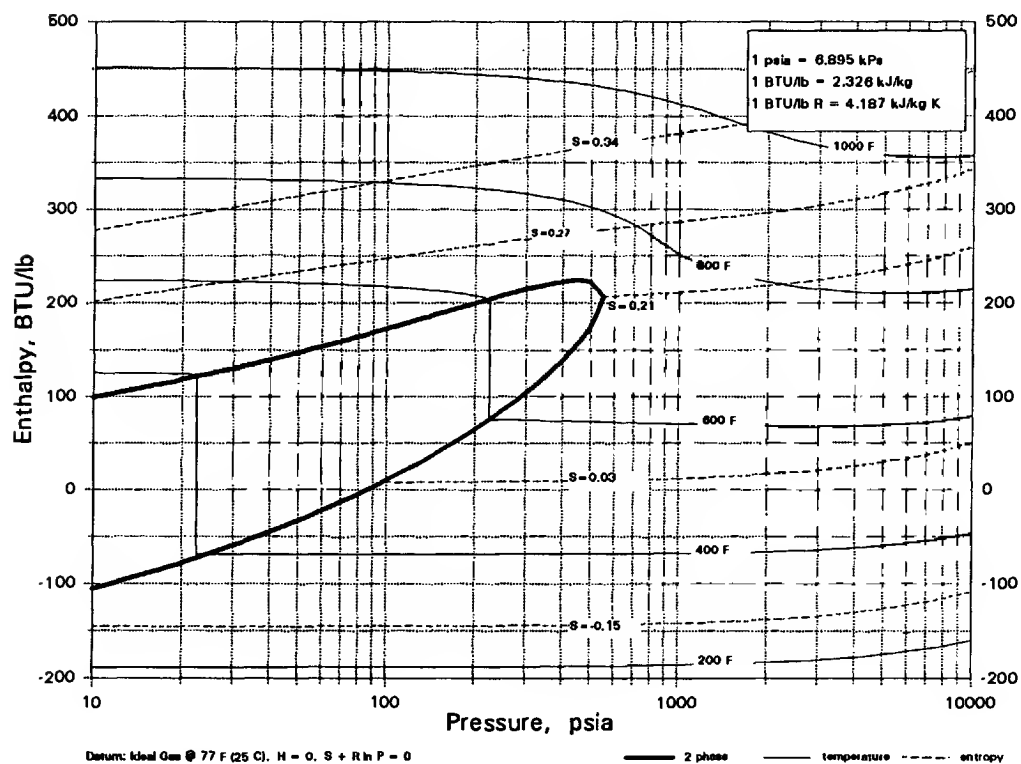
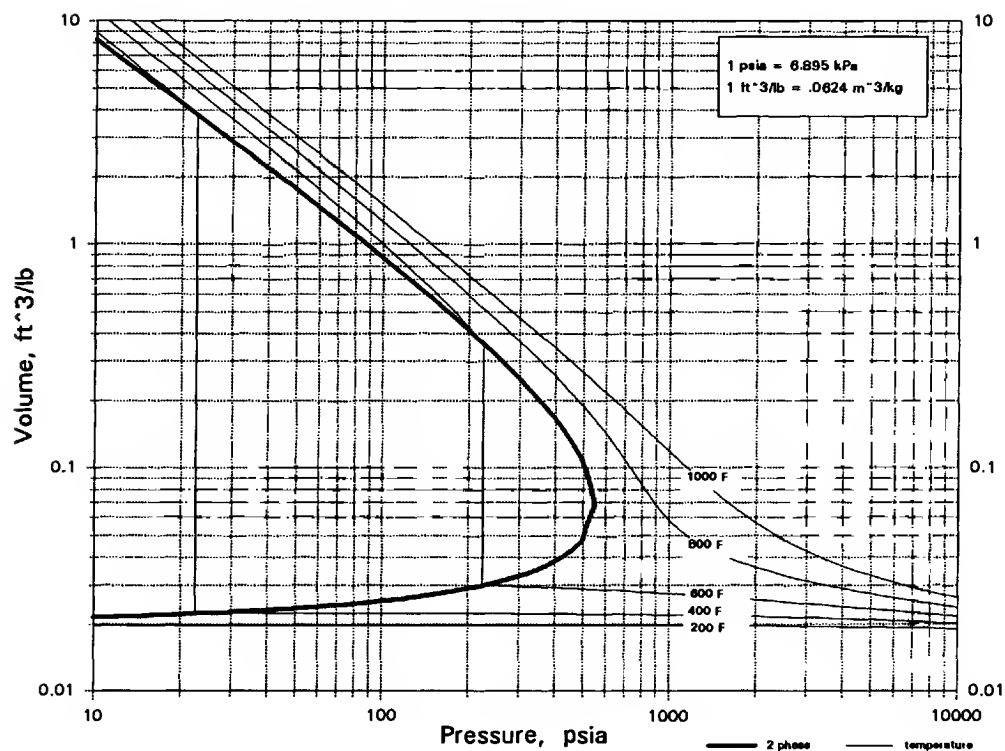
C5H10O2

ISOVALERIC ACID

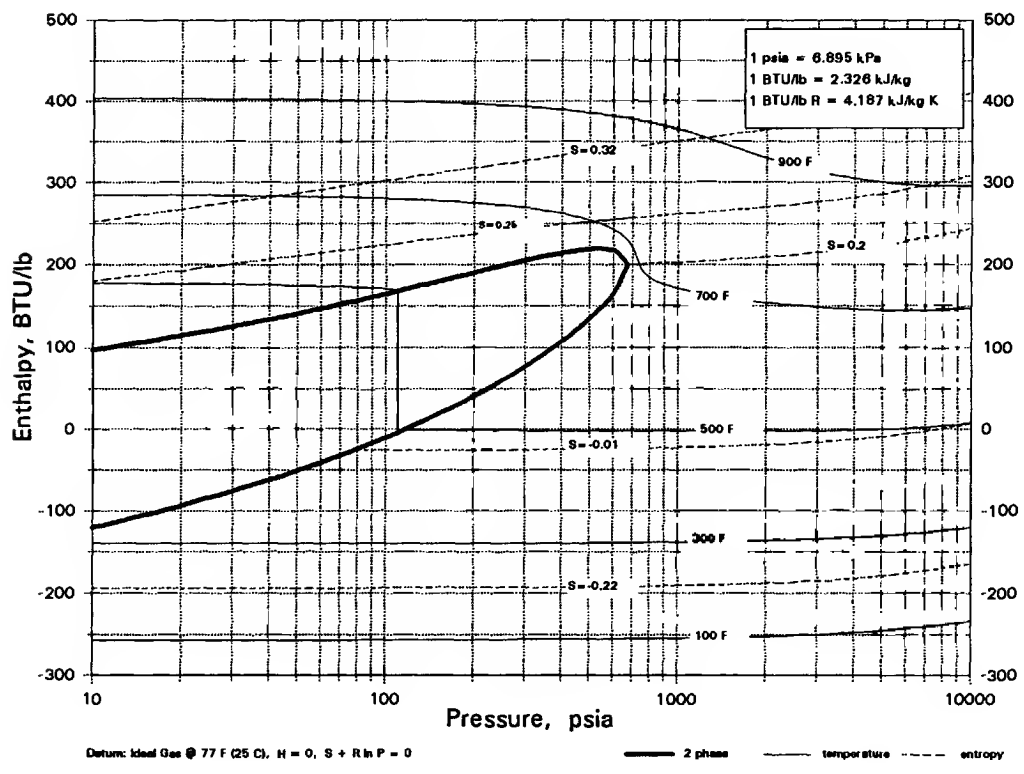
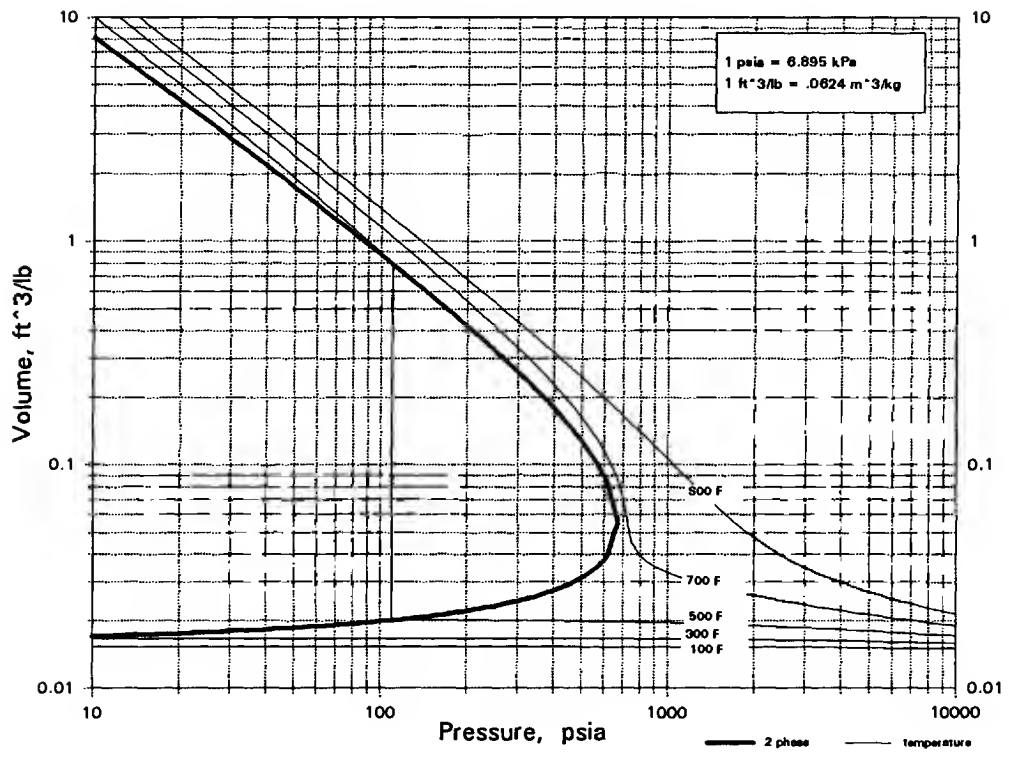


C5H10O2

VALERIC ACID

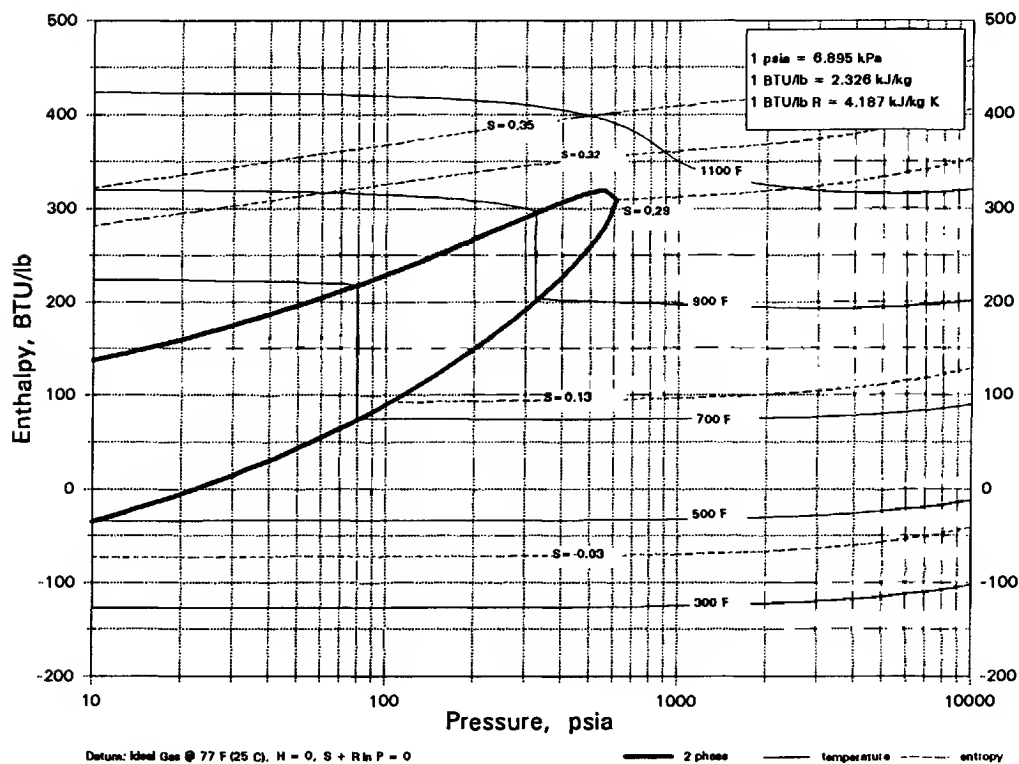
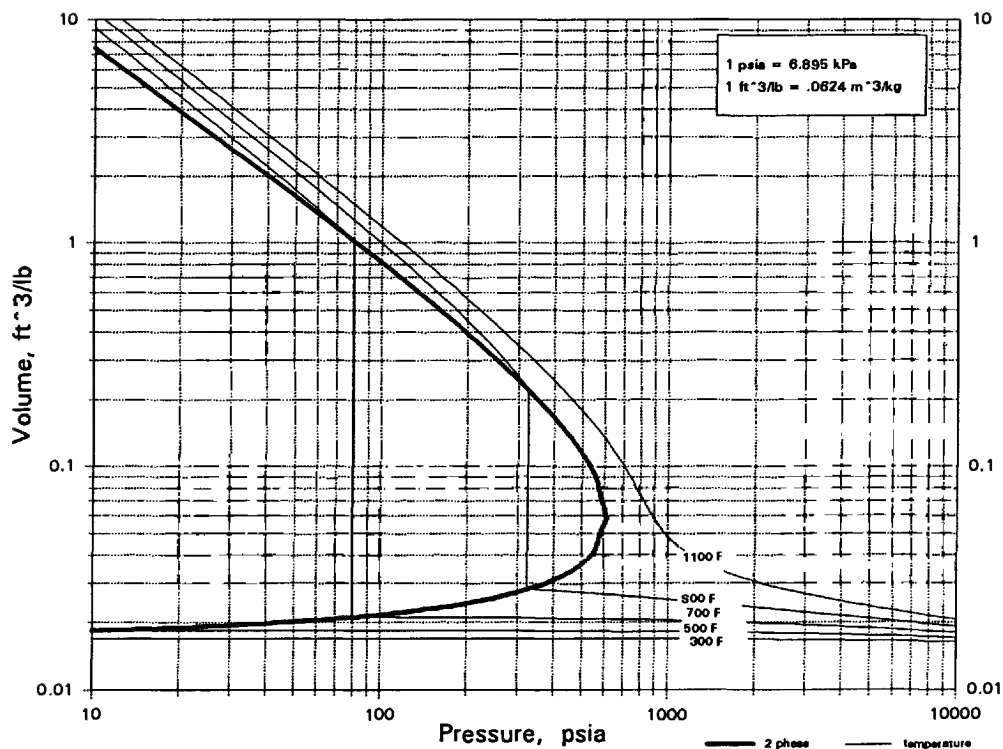


C5H10O2
TETRAHYDROFURFURYL ALCOHOL



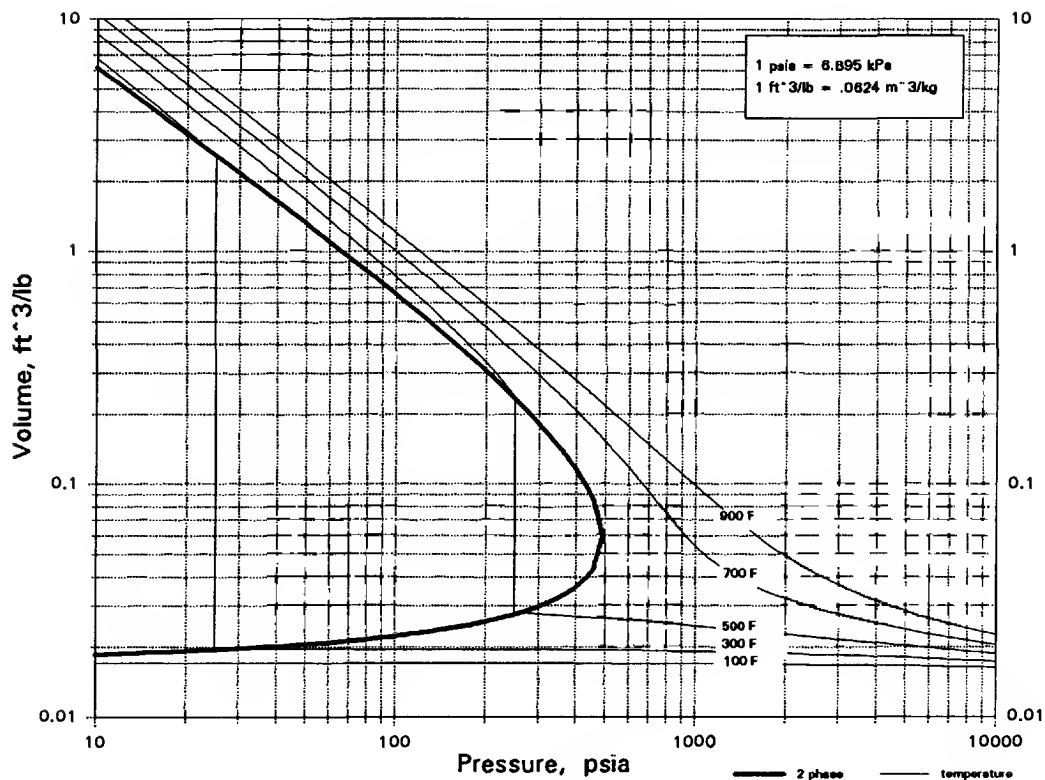
C5H10O2S

3-METHYL SULFOLANE



C5H10O3

DIETHYL CARBONATE



1. Boiling Point, K..... 399.95

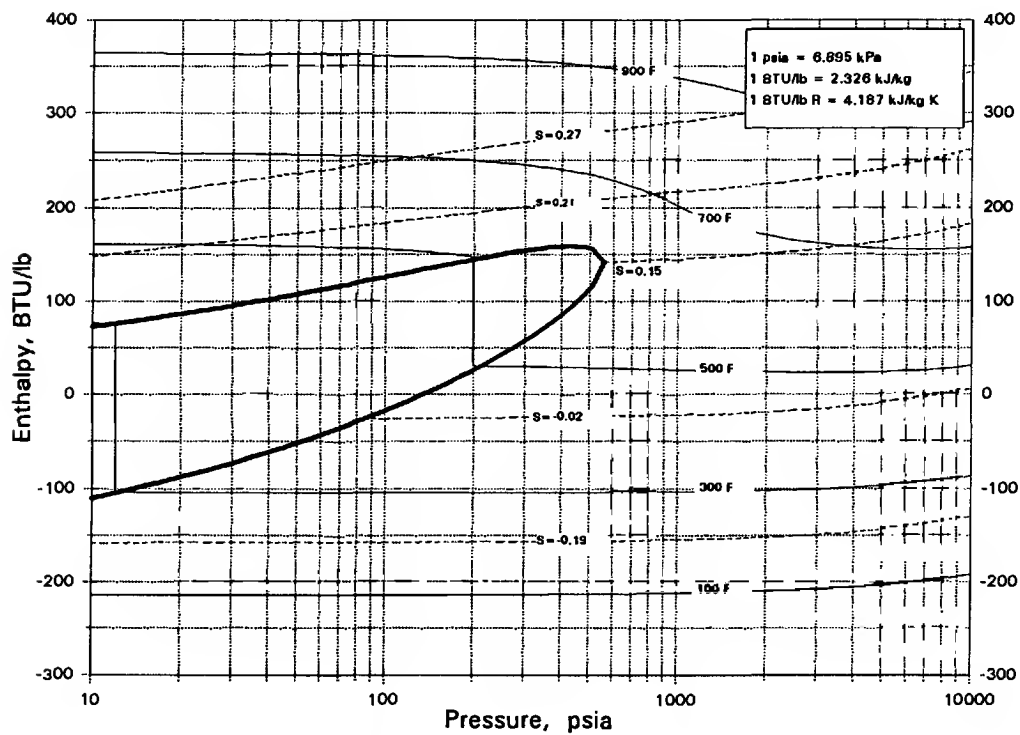
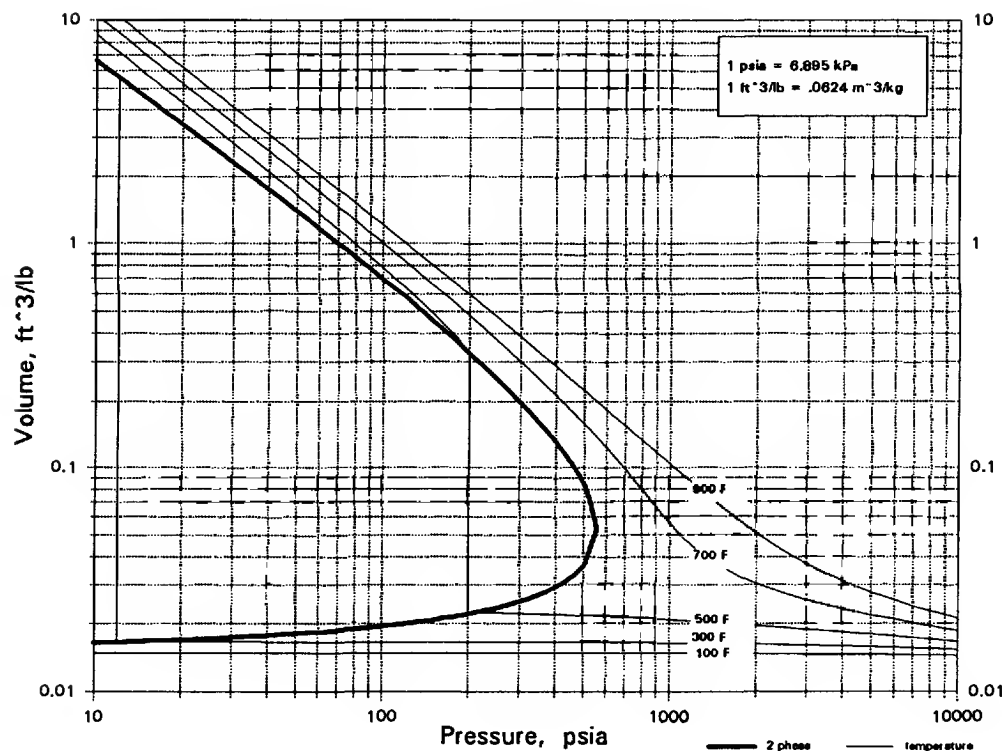
2. Critical Temperature, K.... 576.00

3. Critical Pressure, atm..... 33.46

Heat capacity data are not available.

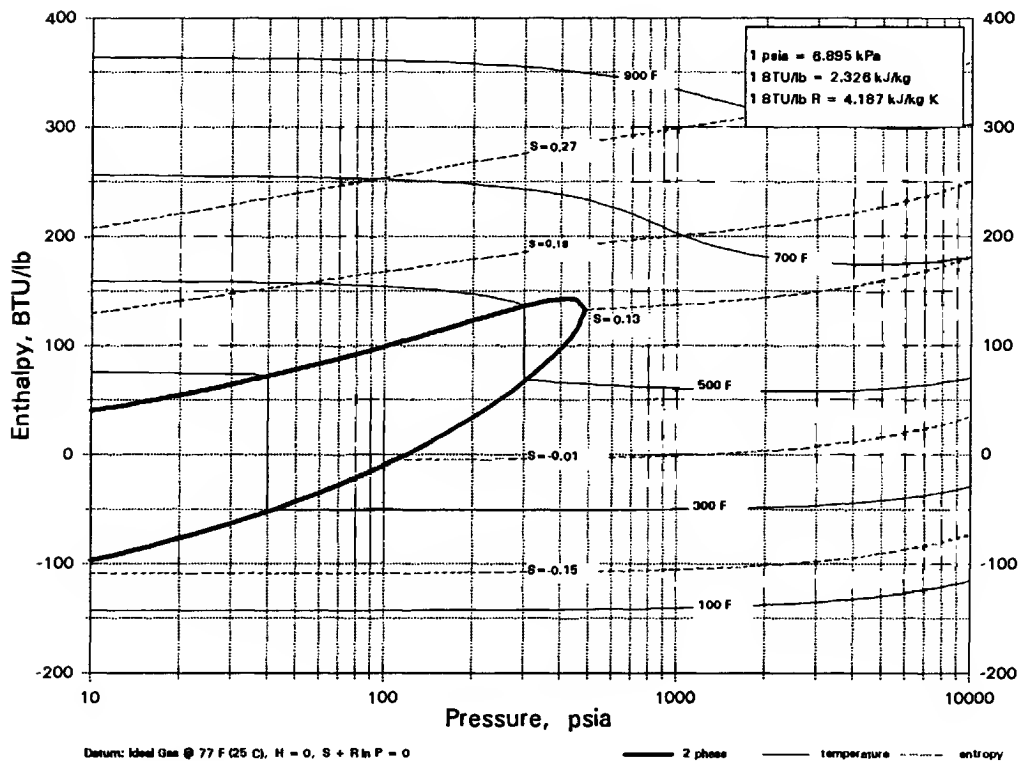
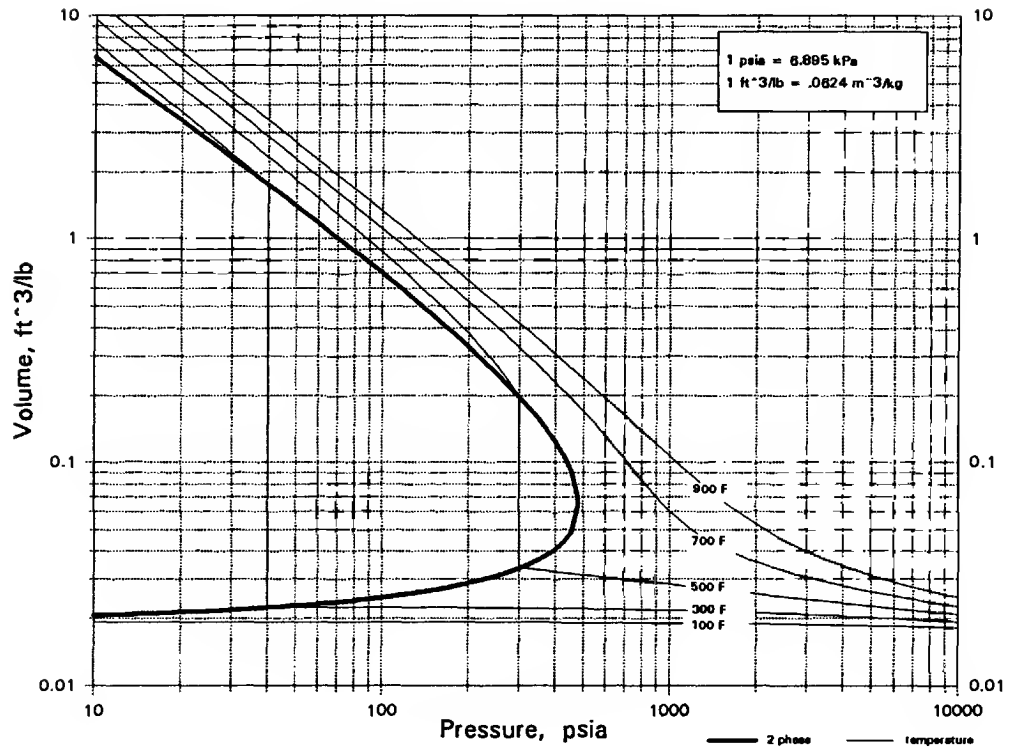
C5H10O3

ETHYL LACTATE

Datum: Ideal Gas @ 77 F (25 C), $H = 0$, $S + R \ln P = 0$

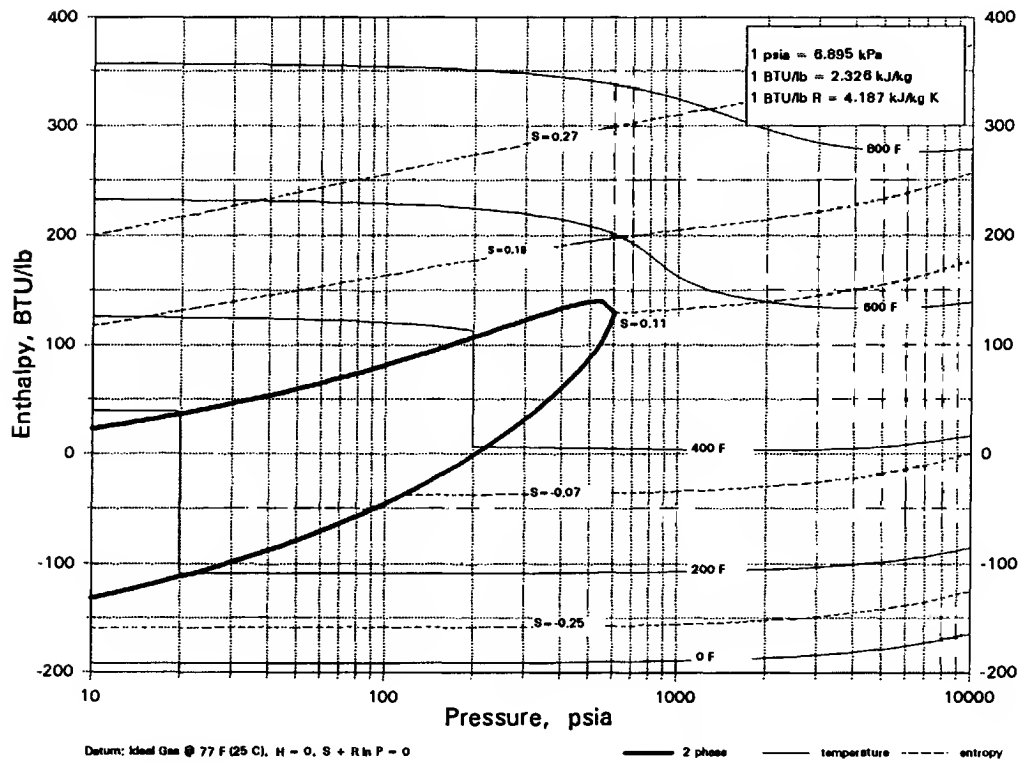
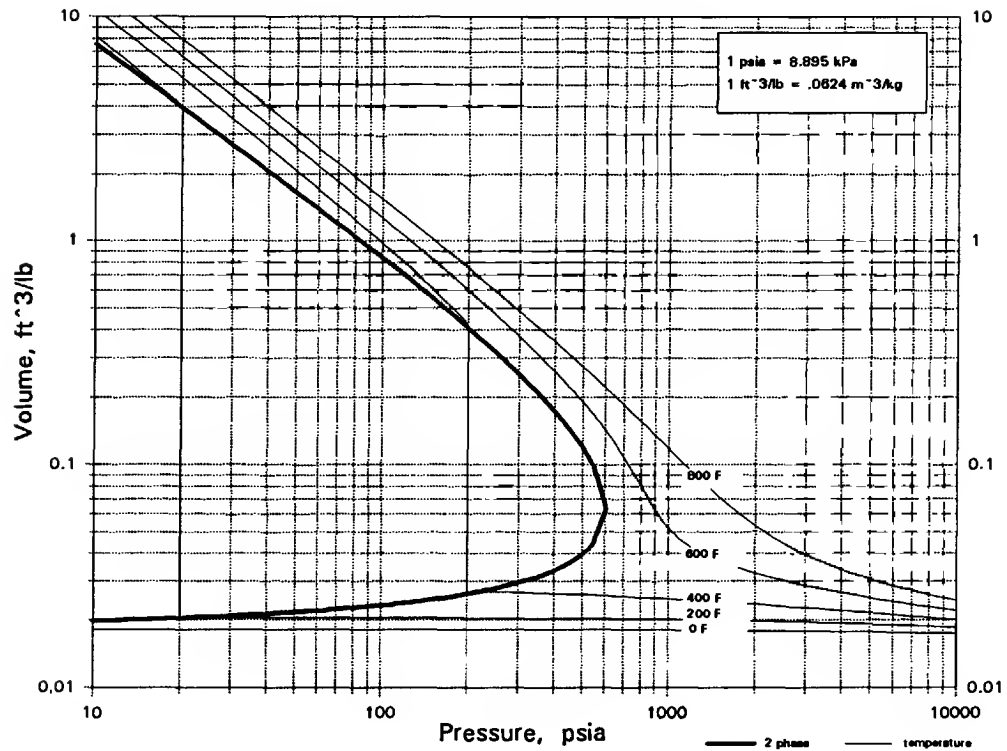
C5H11Cl

1-CHLOROPENTANE



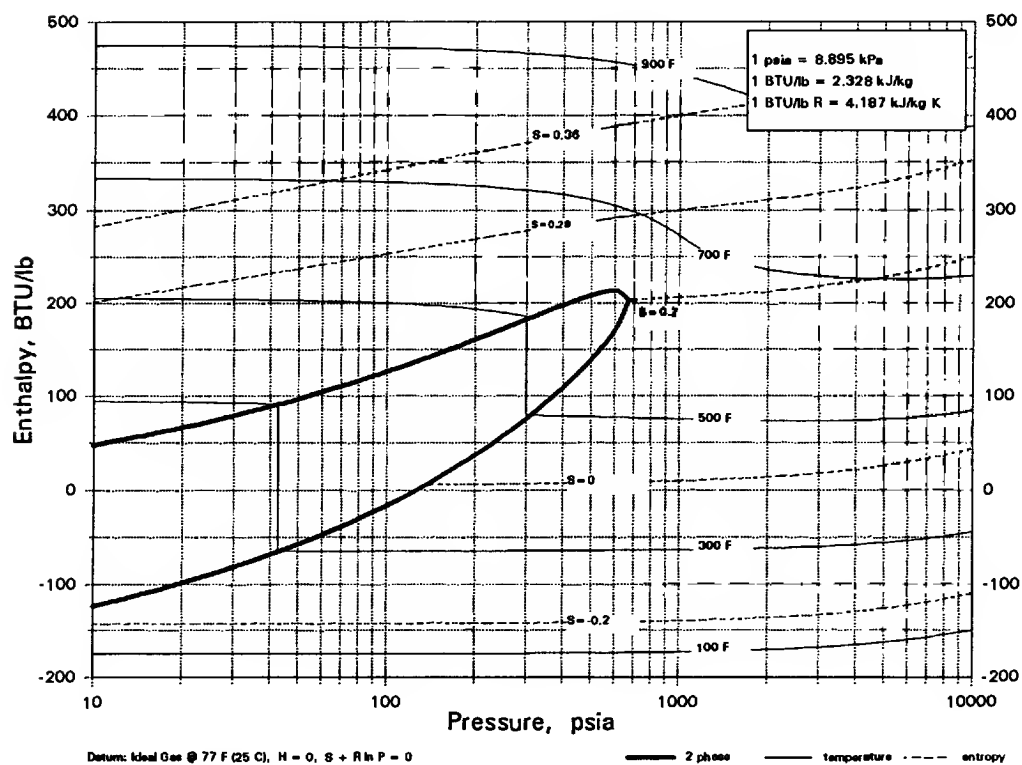
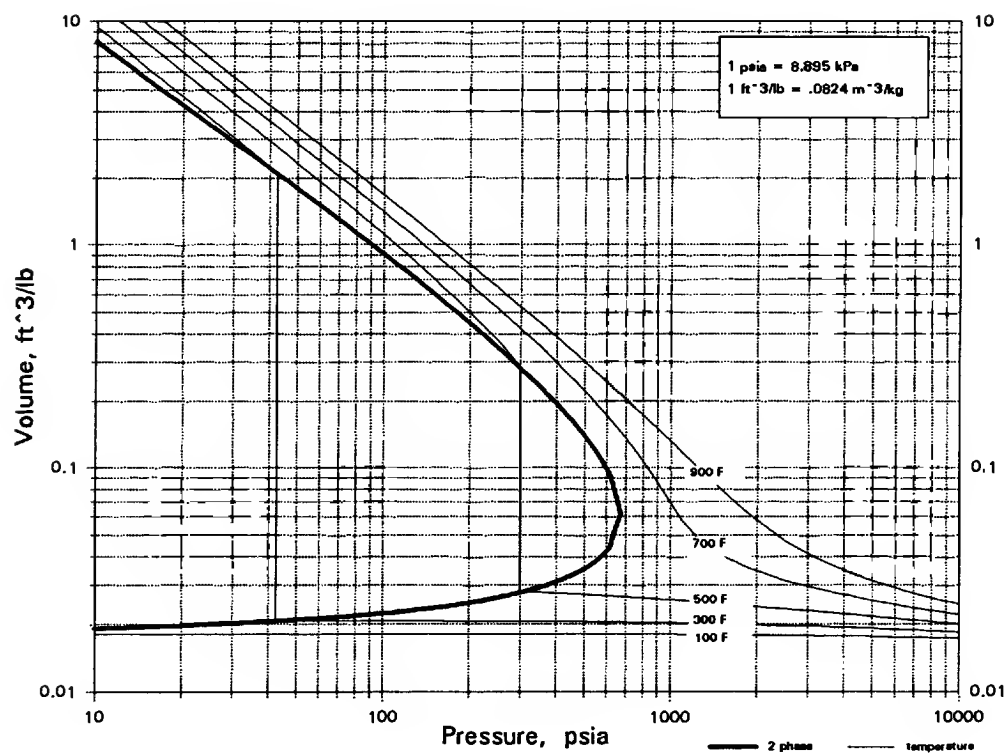
C5H11N

N-METHYLPYRROLIDINE



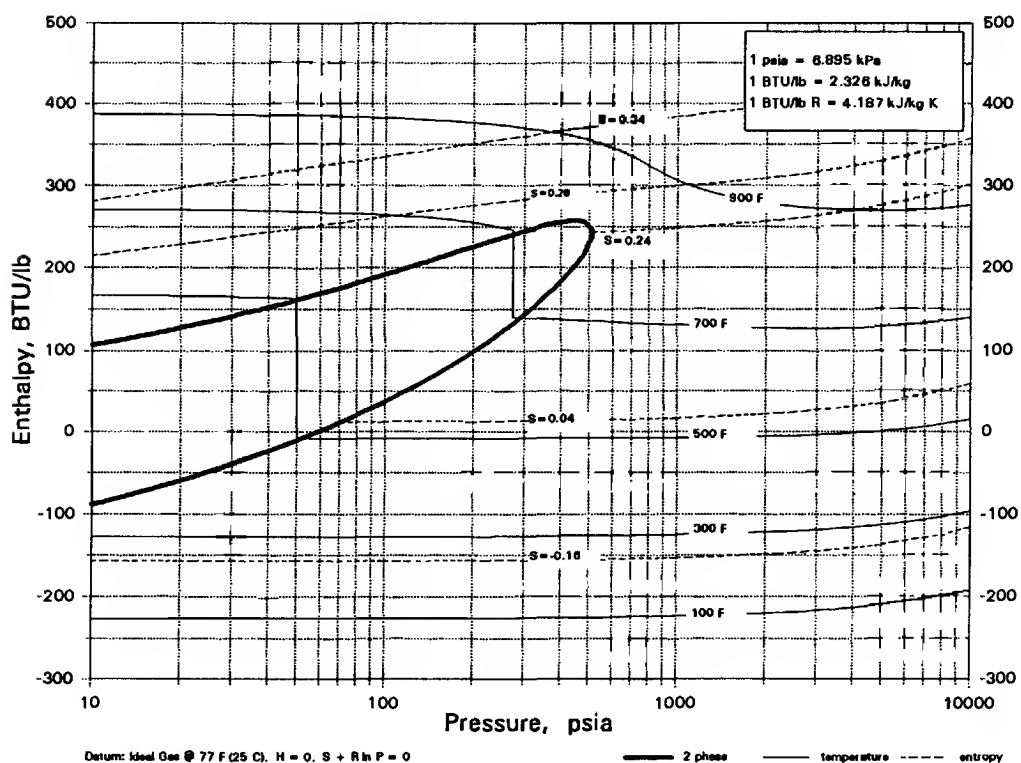
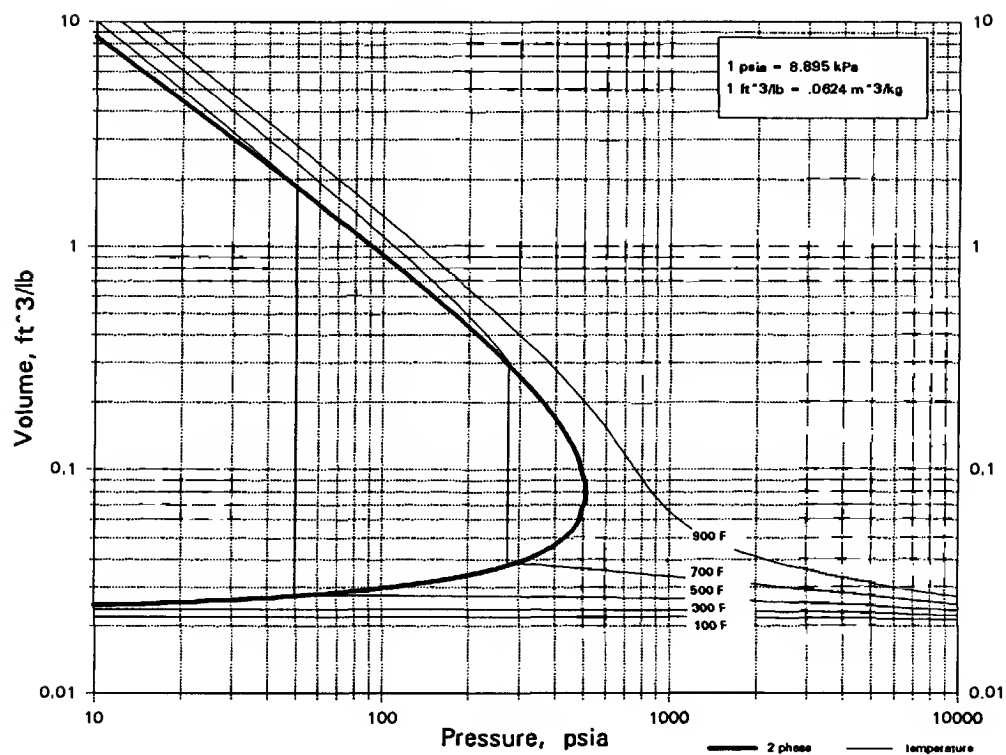
C5H11N

PIPERIDINE



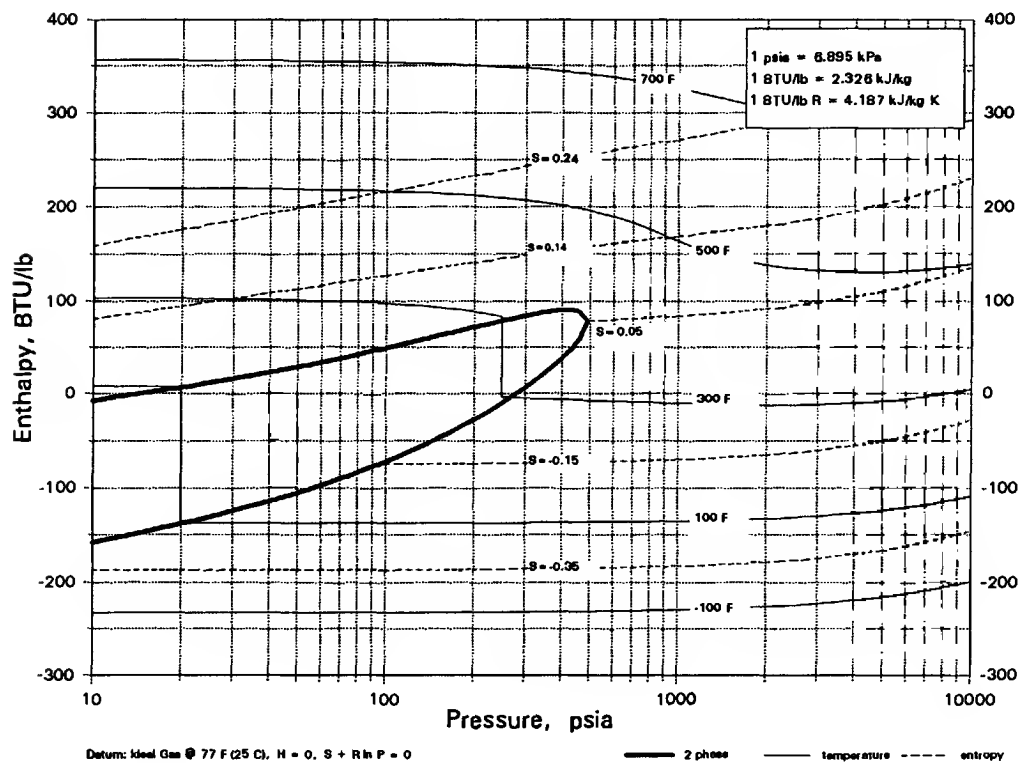
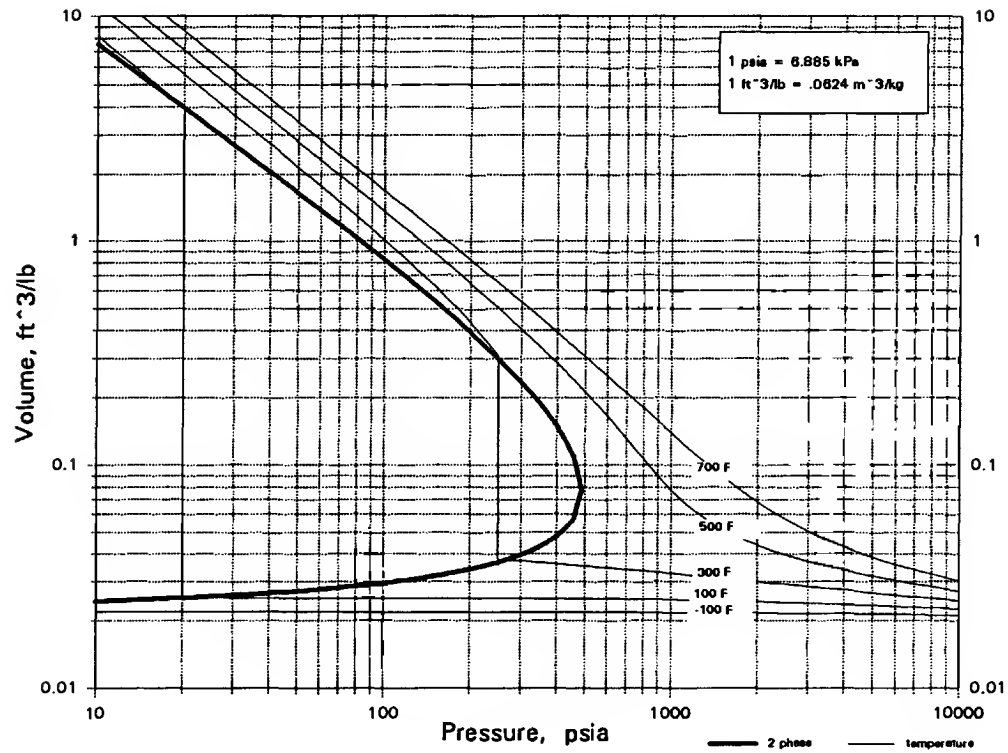
C5H11NO

tert-BUTYLFORMAMIDE



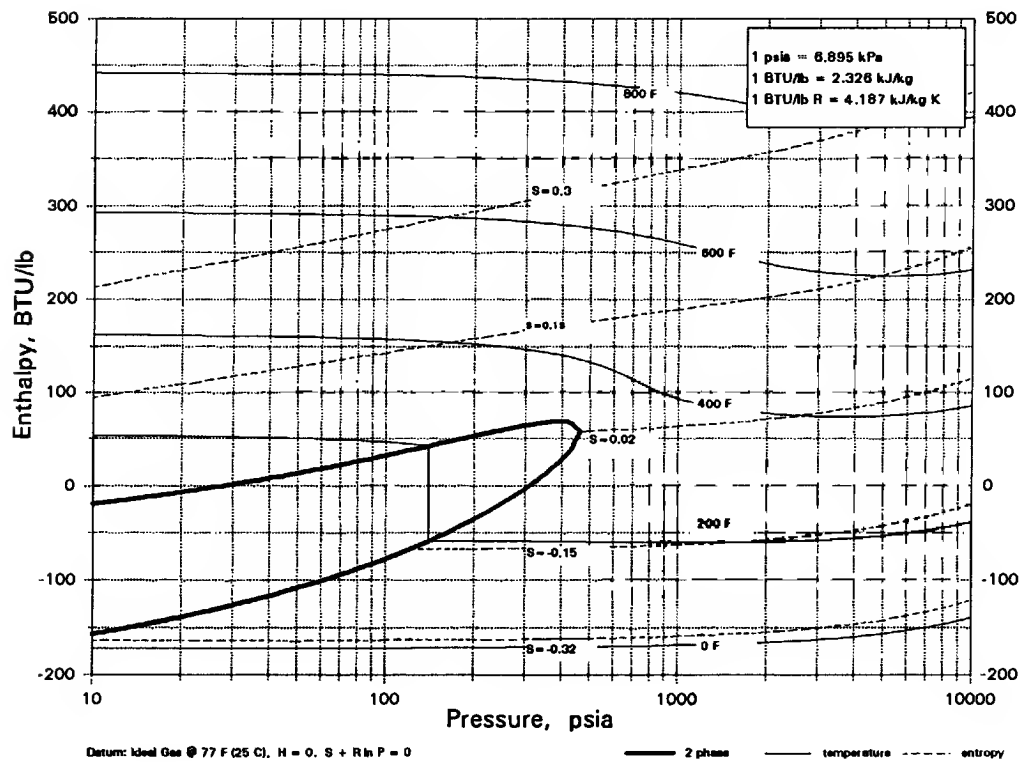
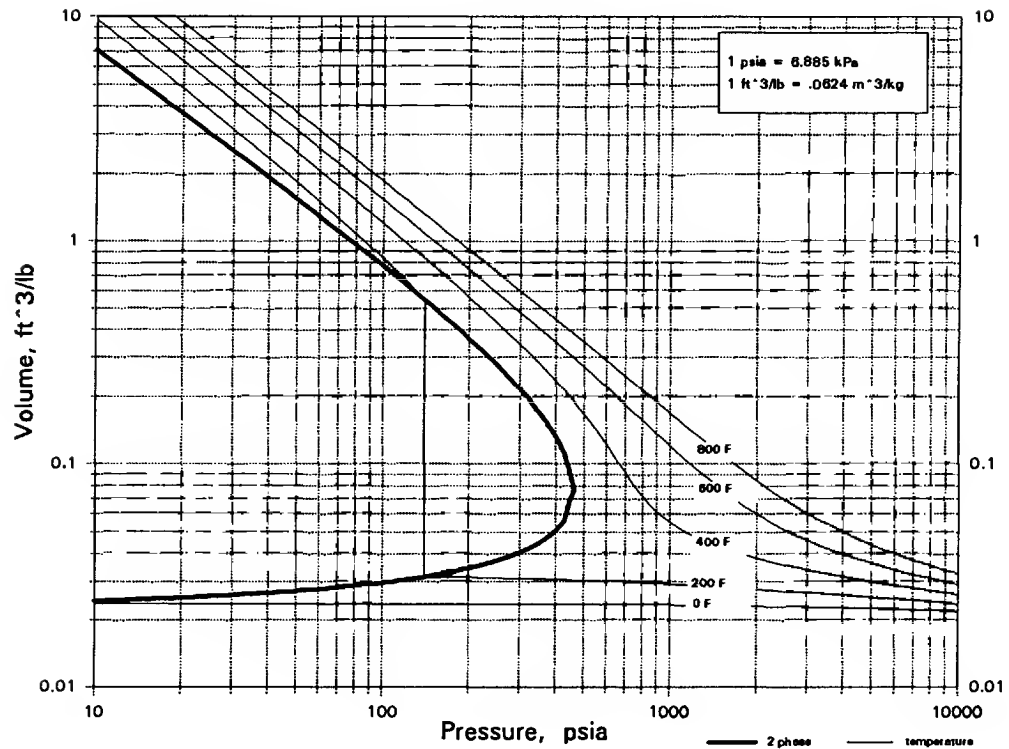
C5H12

ISOPENTANE



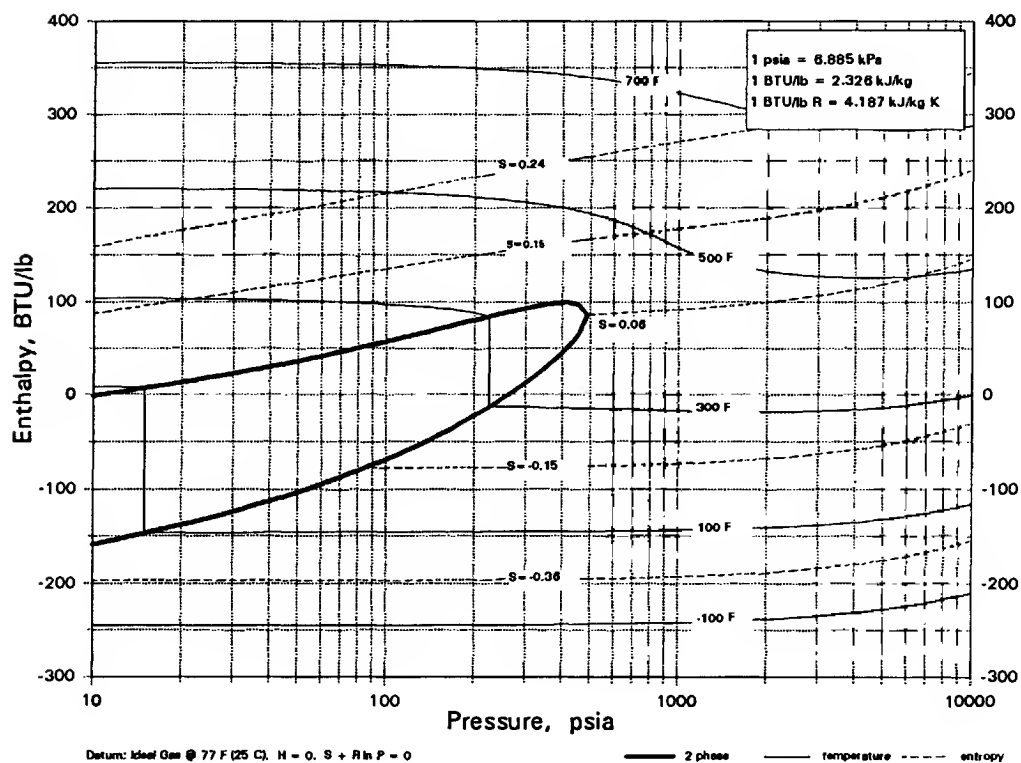
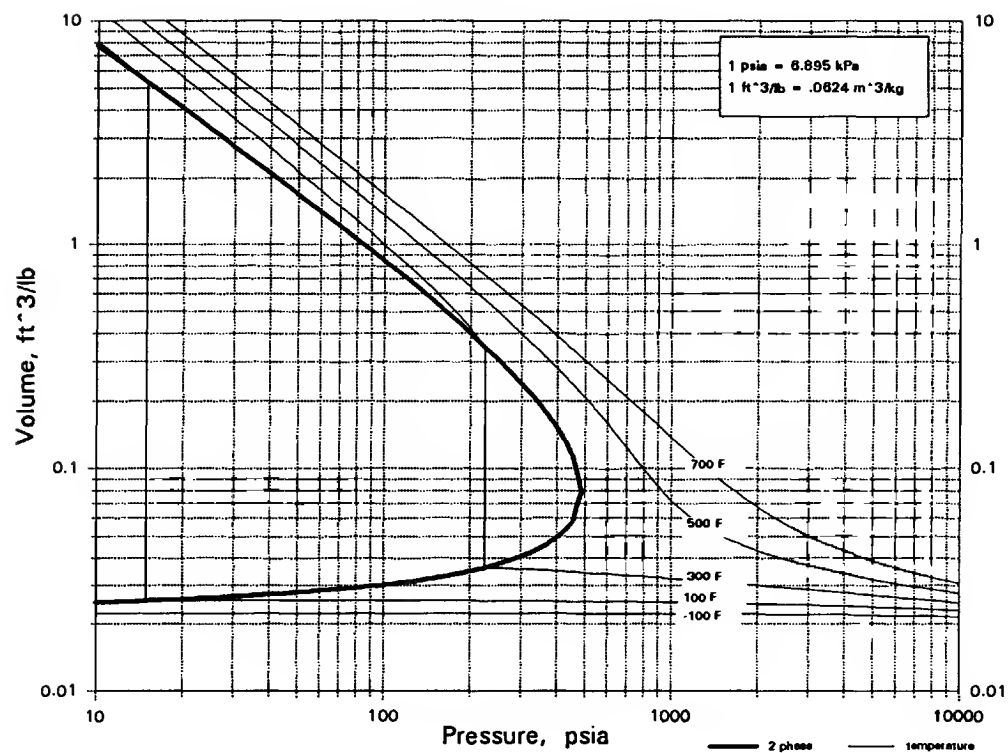
C5H12

NEOPENTANE



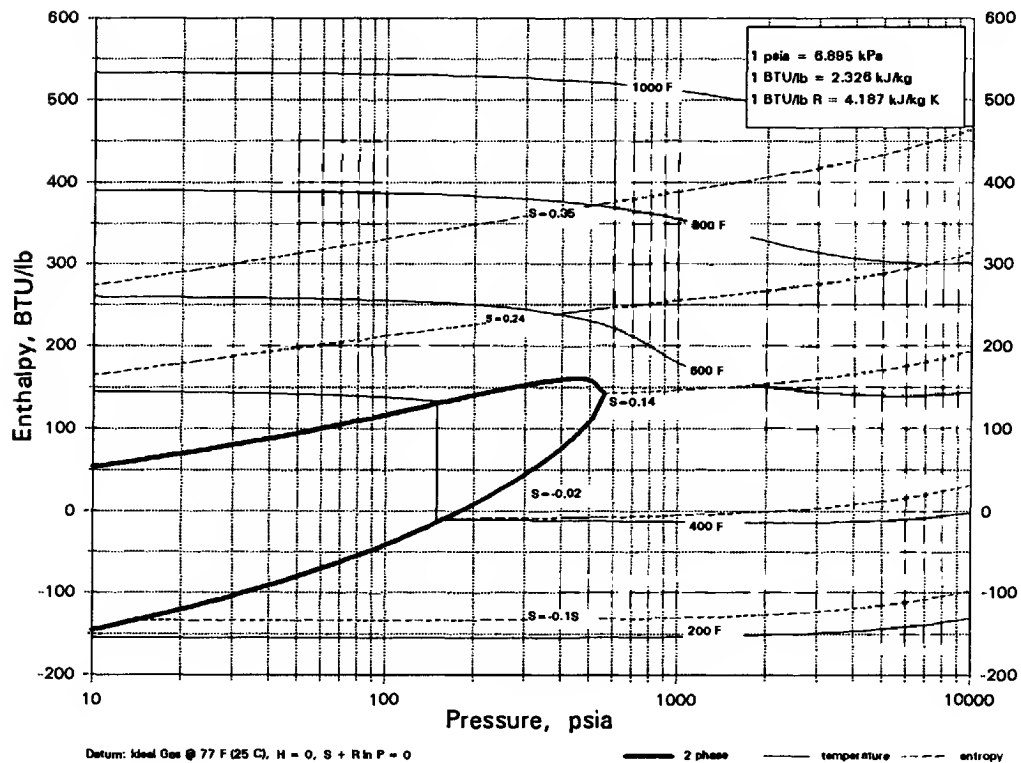
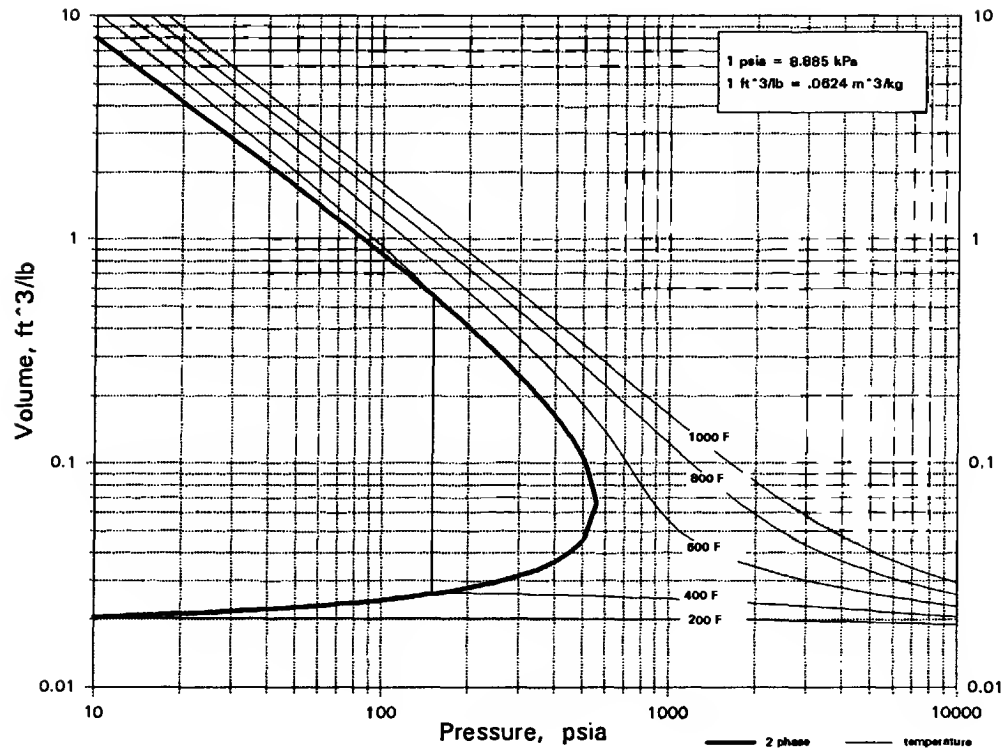
C5H12

n-PENTANE



C5H12O

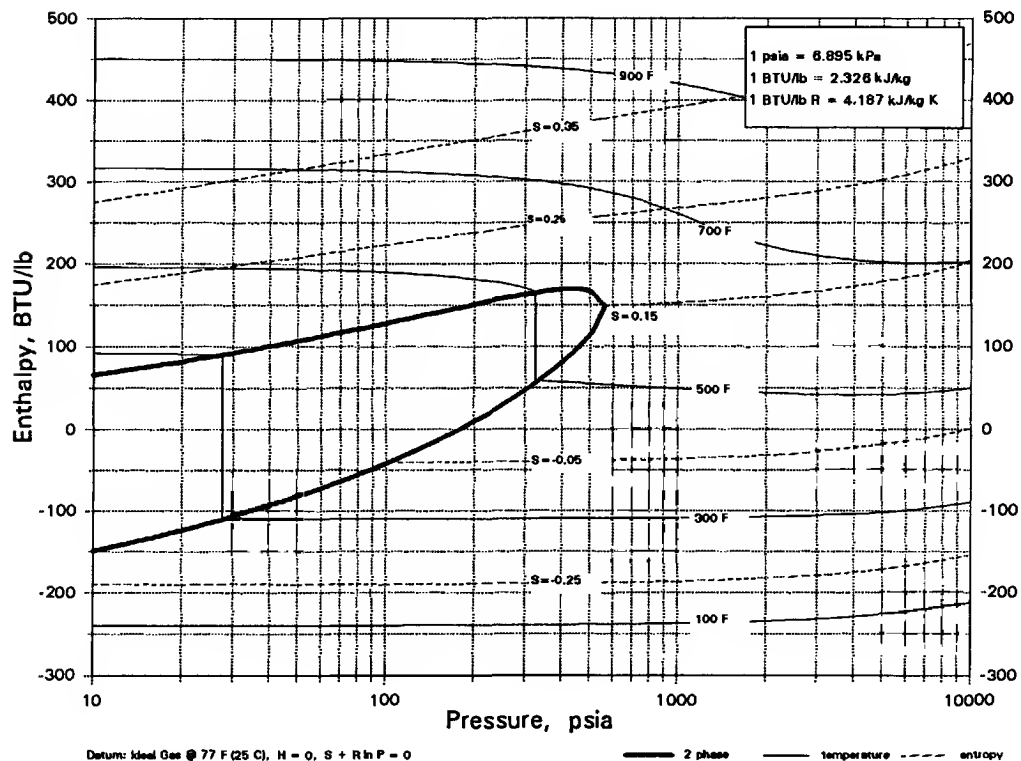
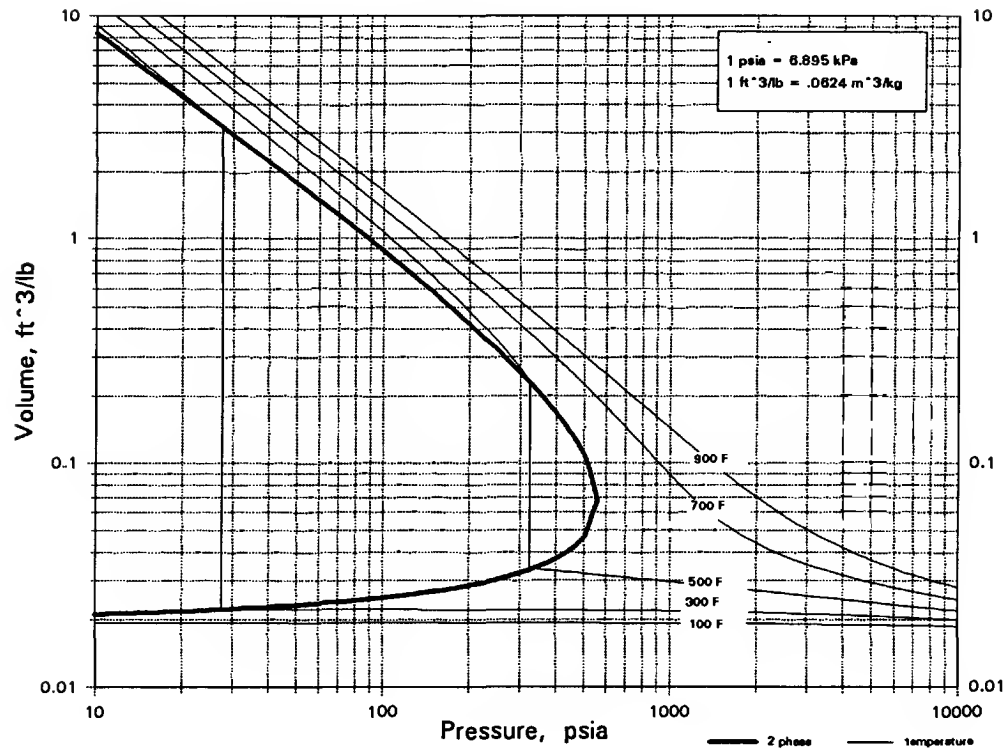
2-2-DIMETHYL-1-PROPANOL



Return: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

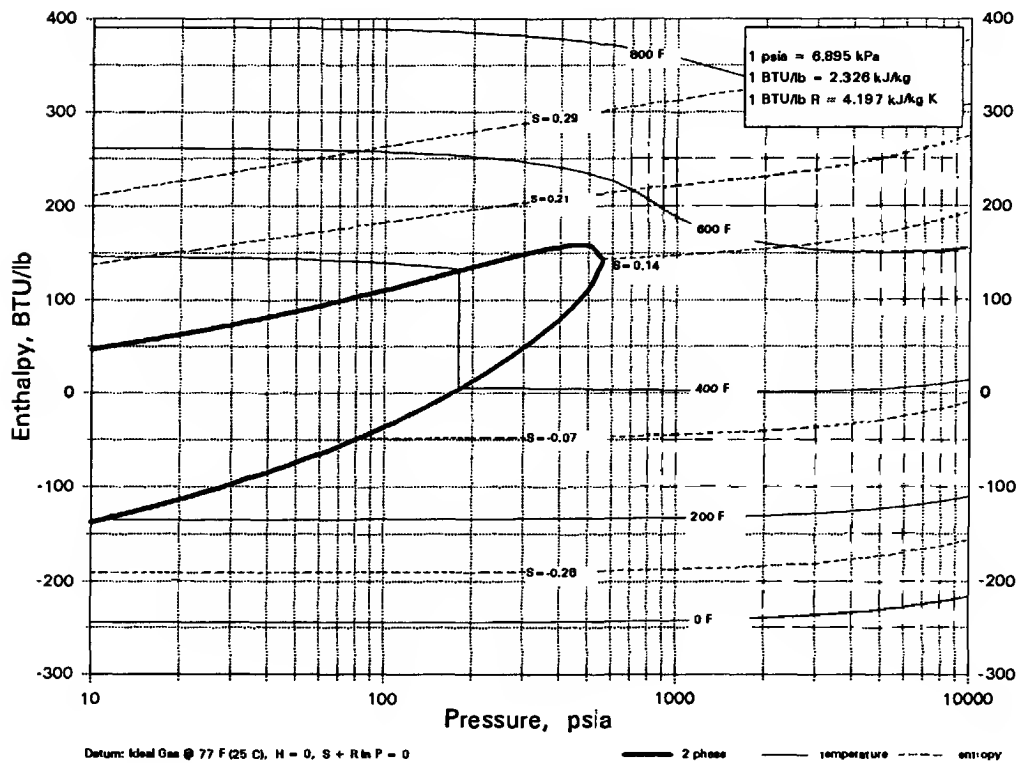
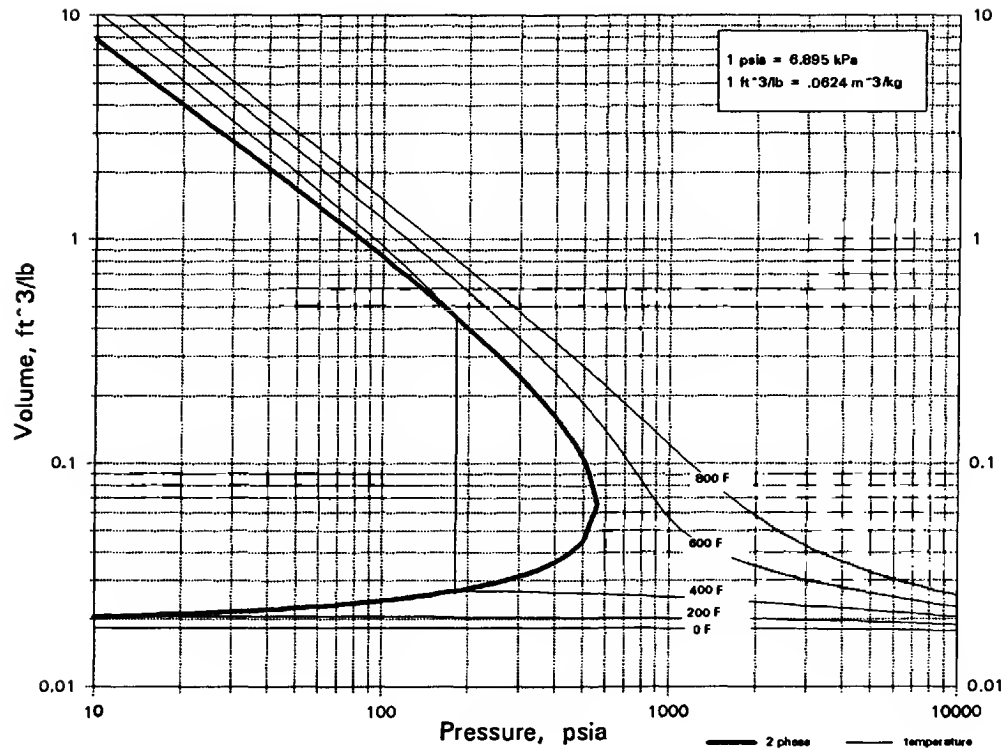
C5H12O

2-METHYL-1-BUTANOL



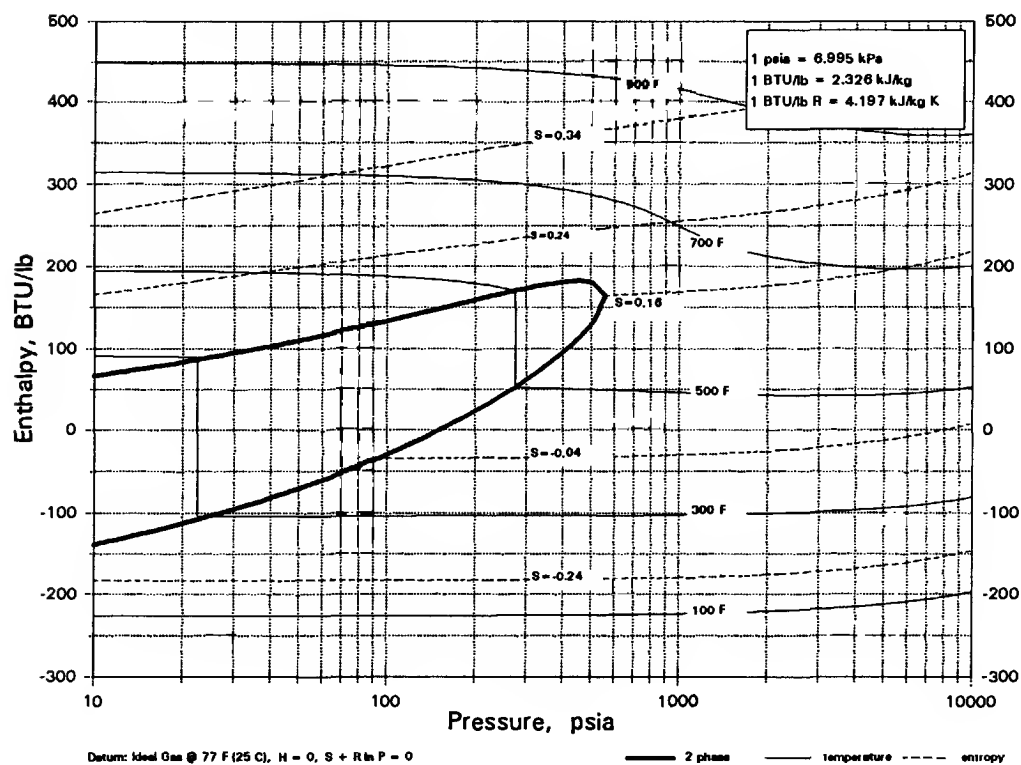
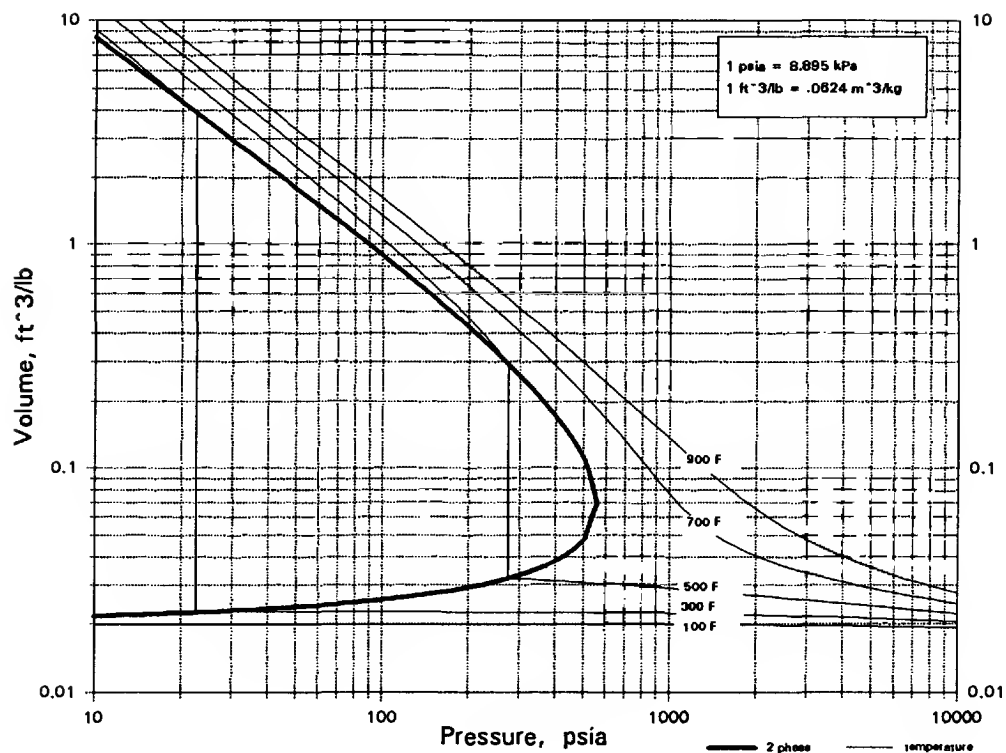
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2-METHYL-2-BUTANOL



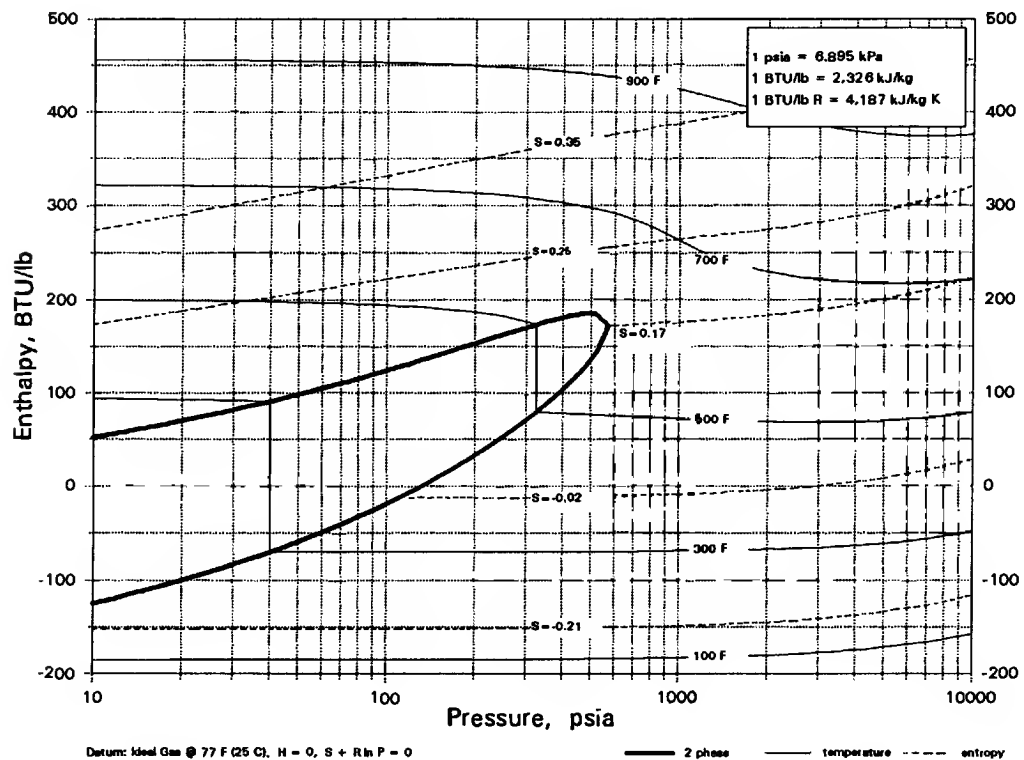
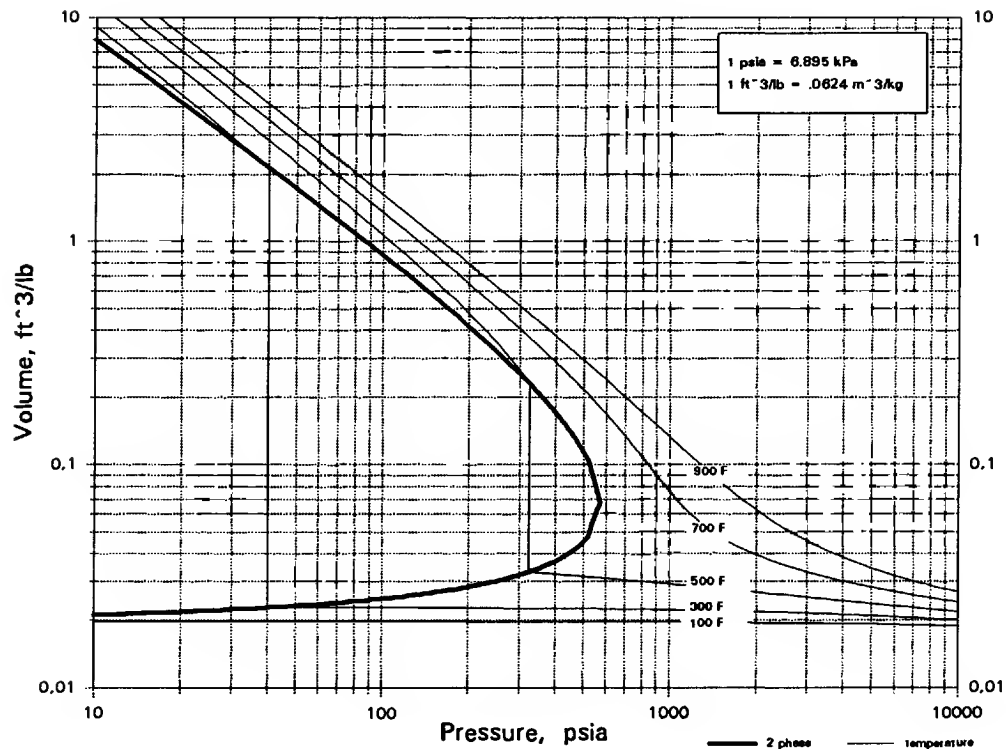
C5H12O

3-METHYL-1-BUTANOL



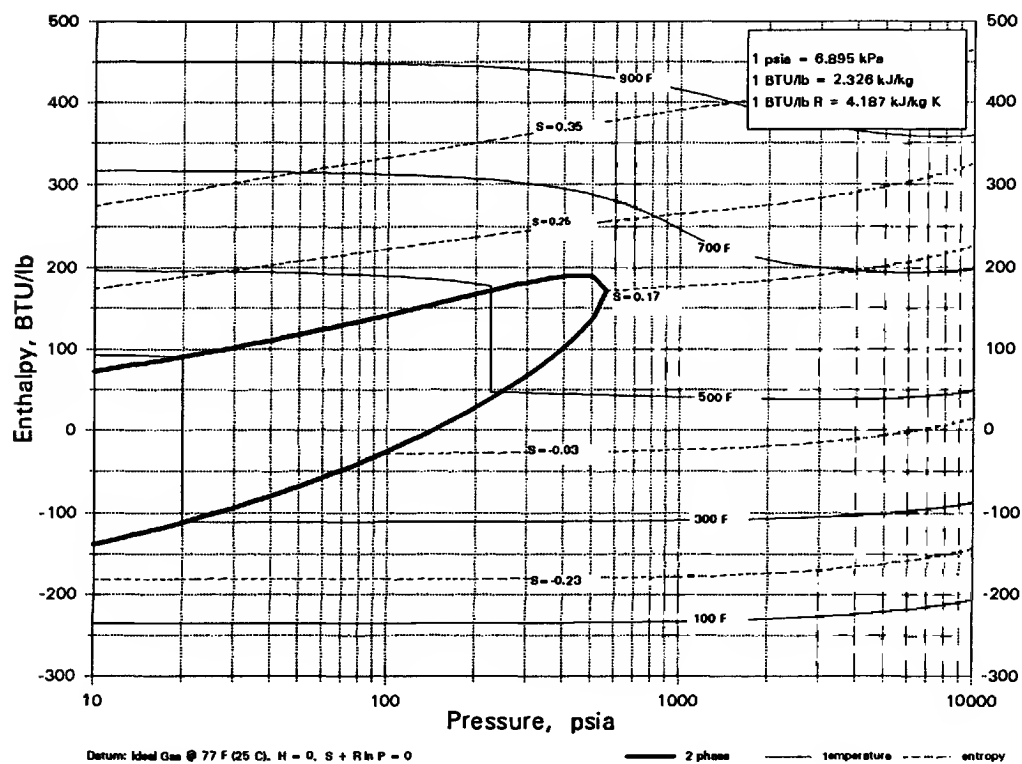
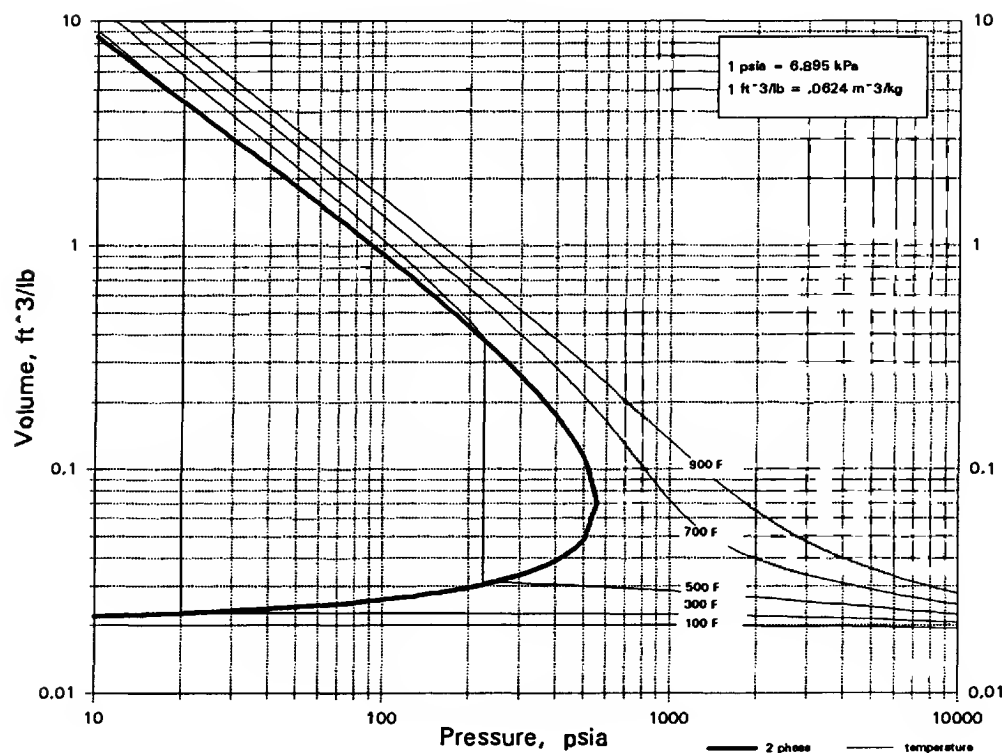
C5H12O

3-METHYL-2-BUTANOL

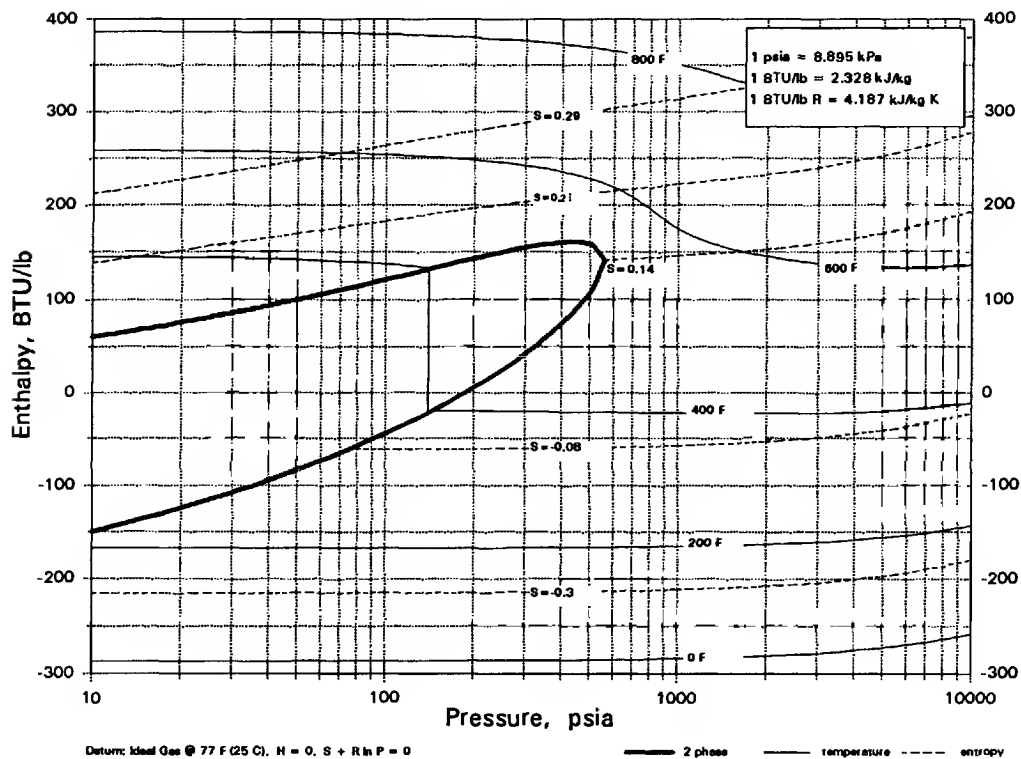
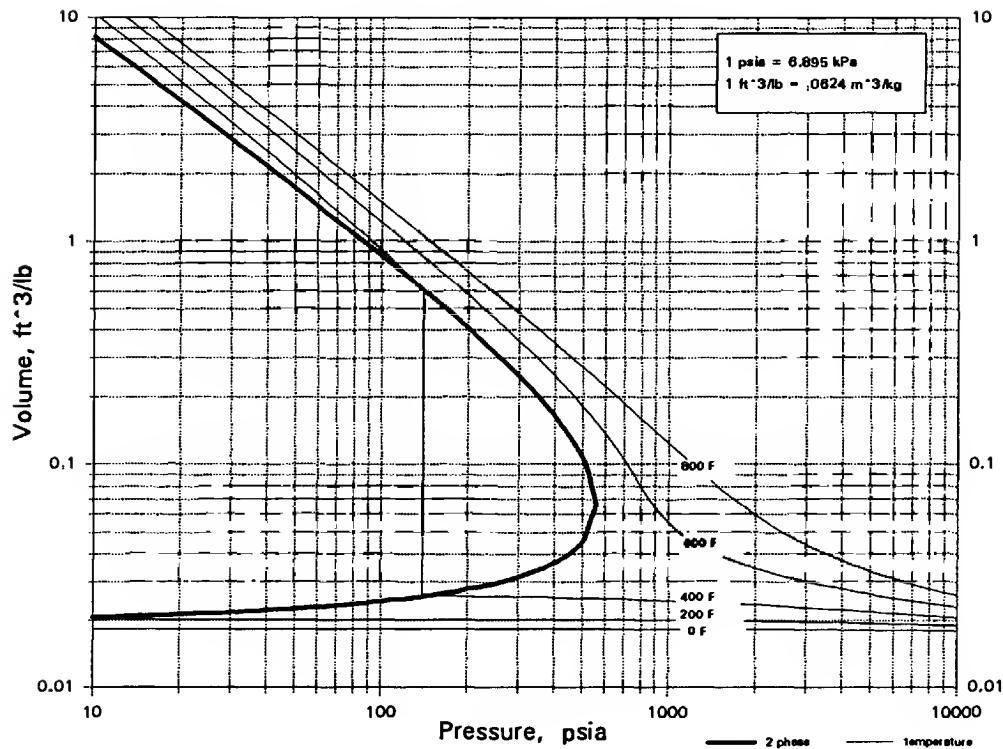


C5H12O

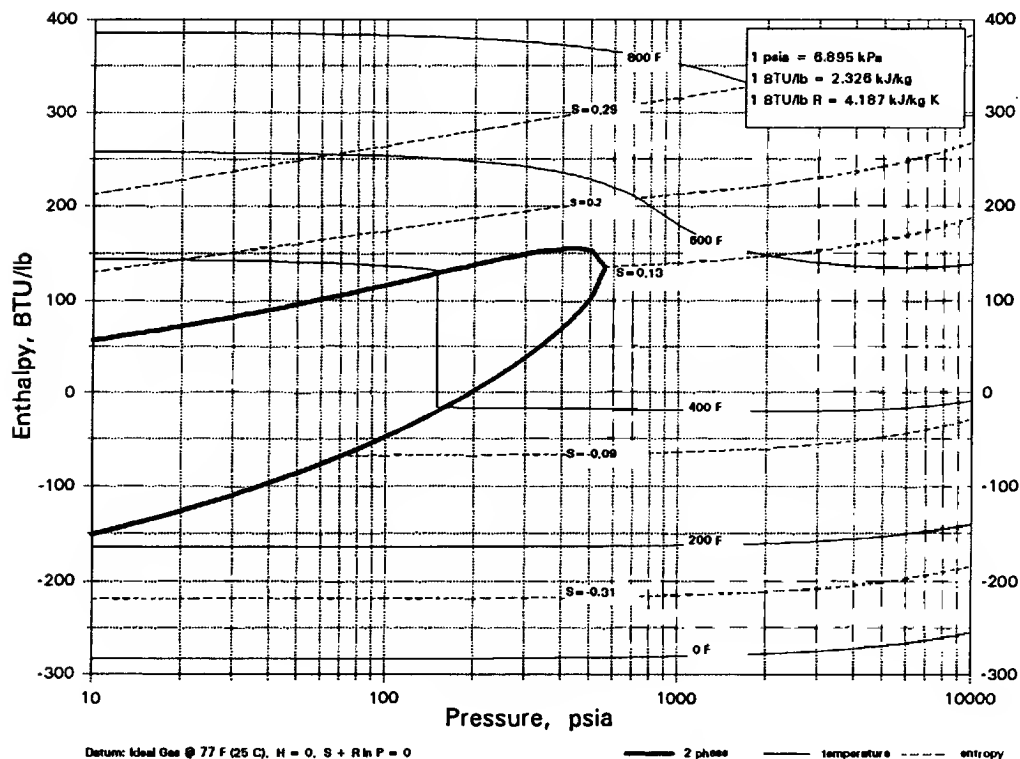
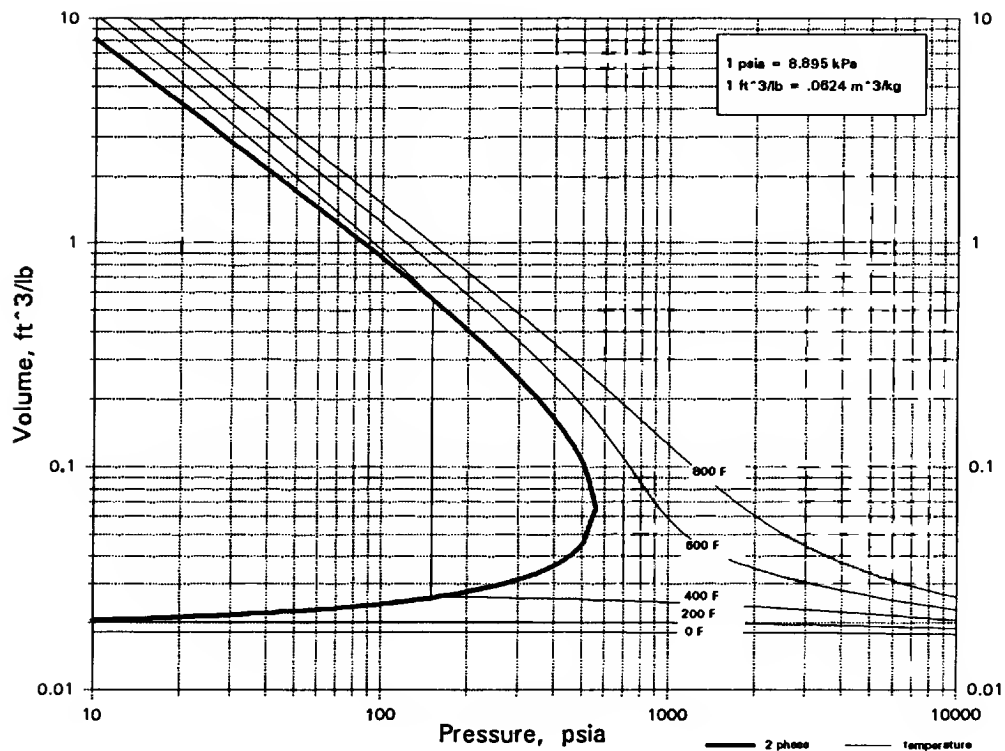
1-PENTANOL



C5H12O
2-PENTANOL

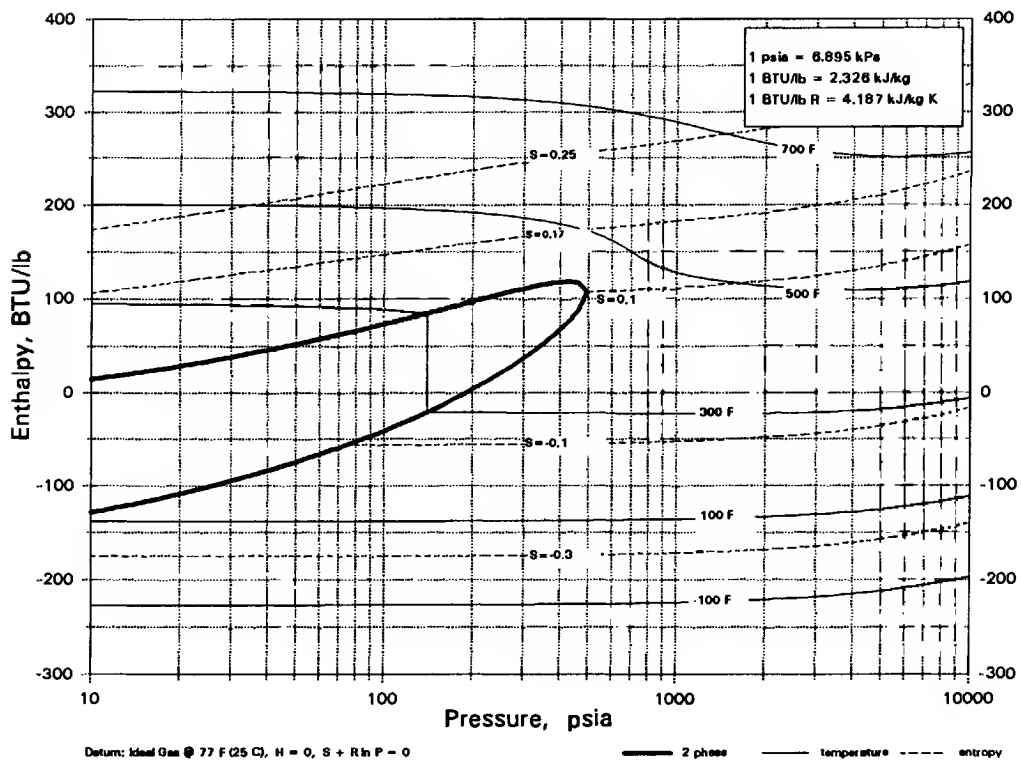
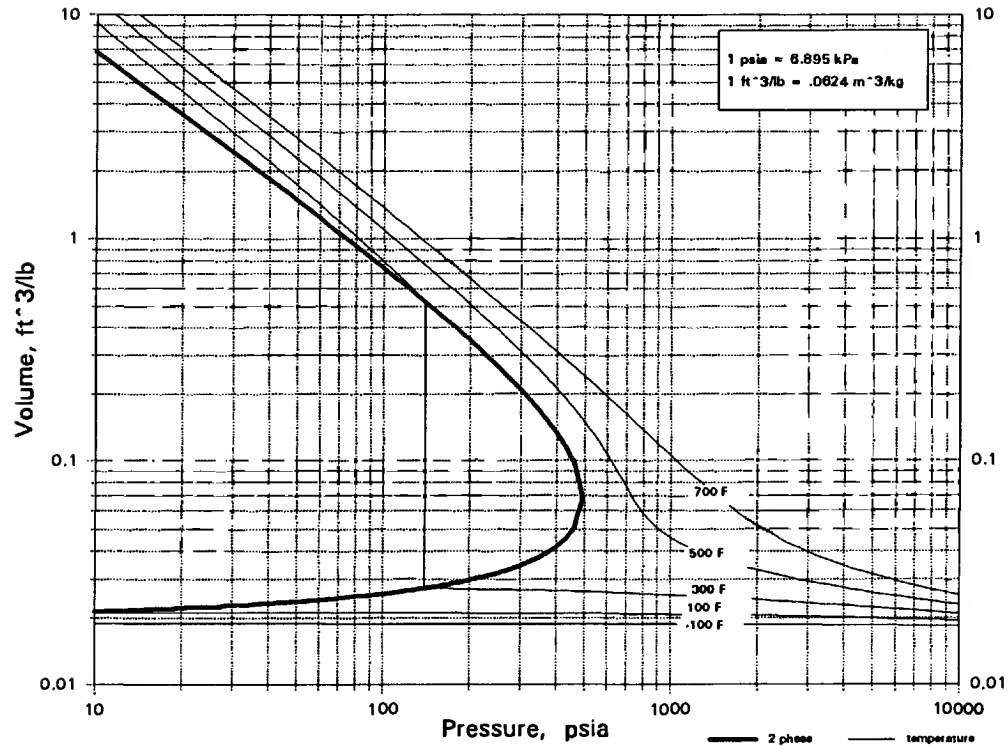


C5H12O
3-PENTANOL



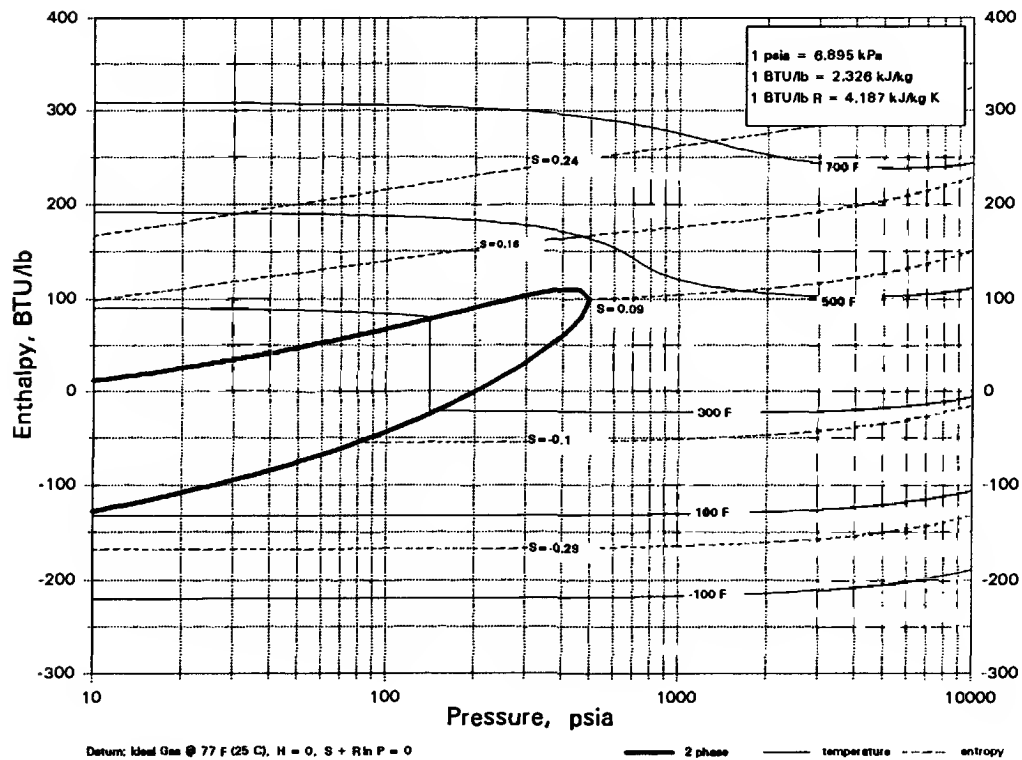
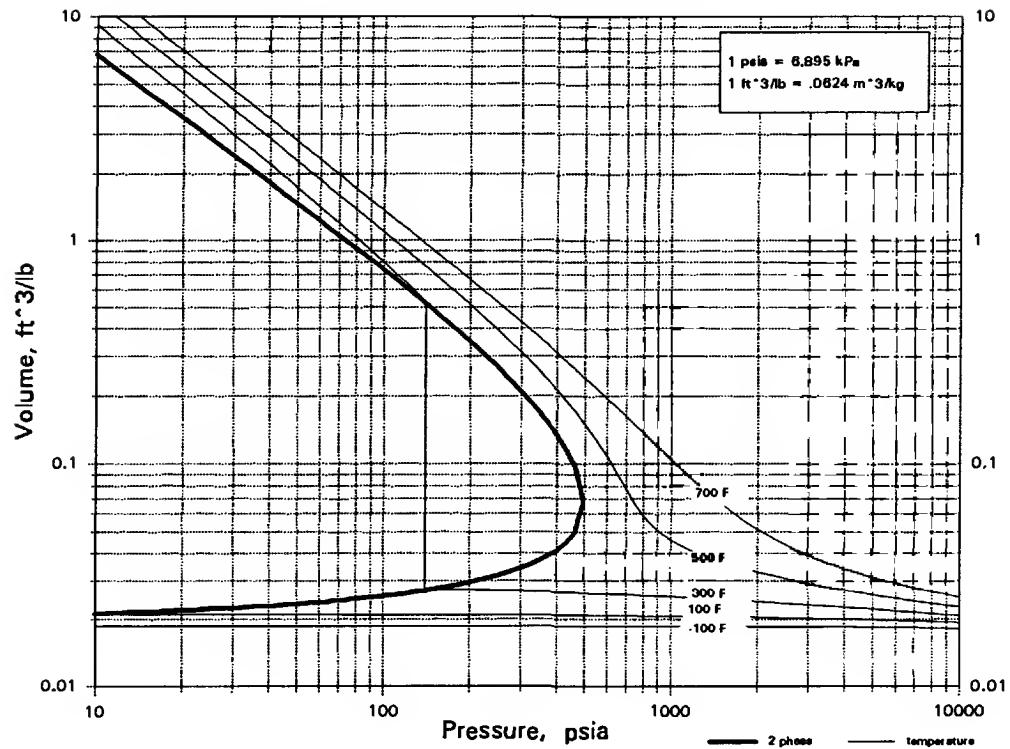
C5H12O

METHYL sec-BUTYL ETHER



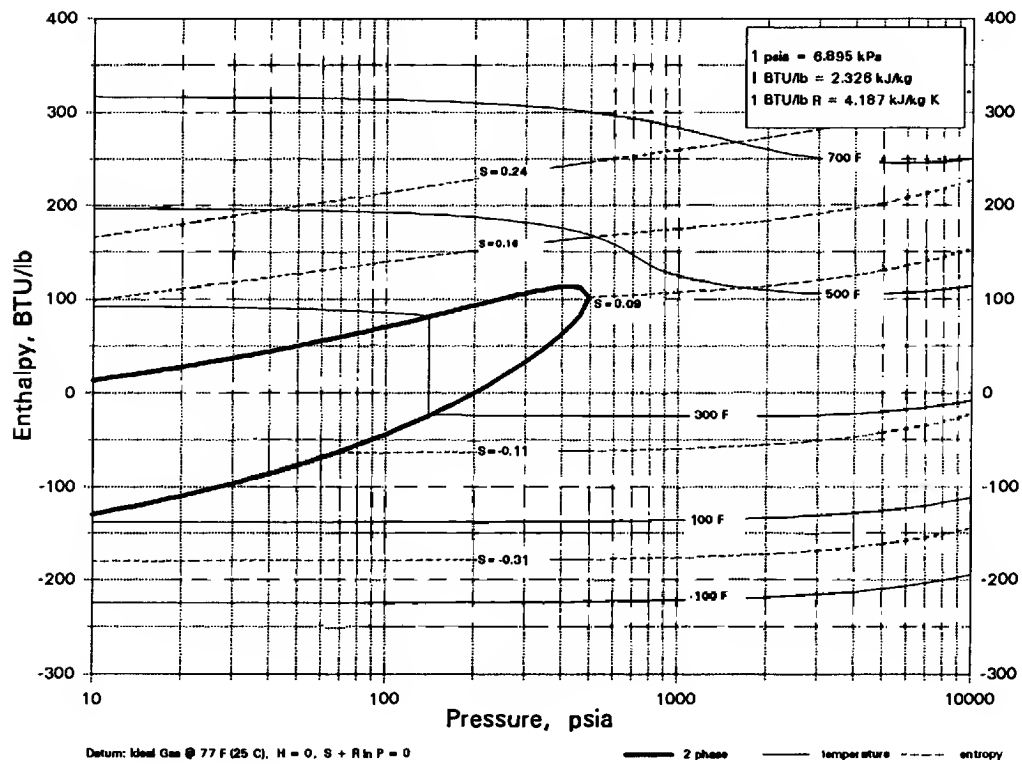
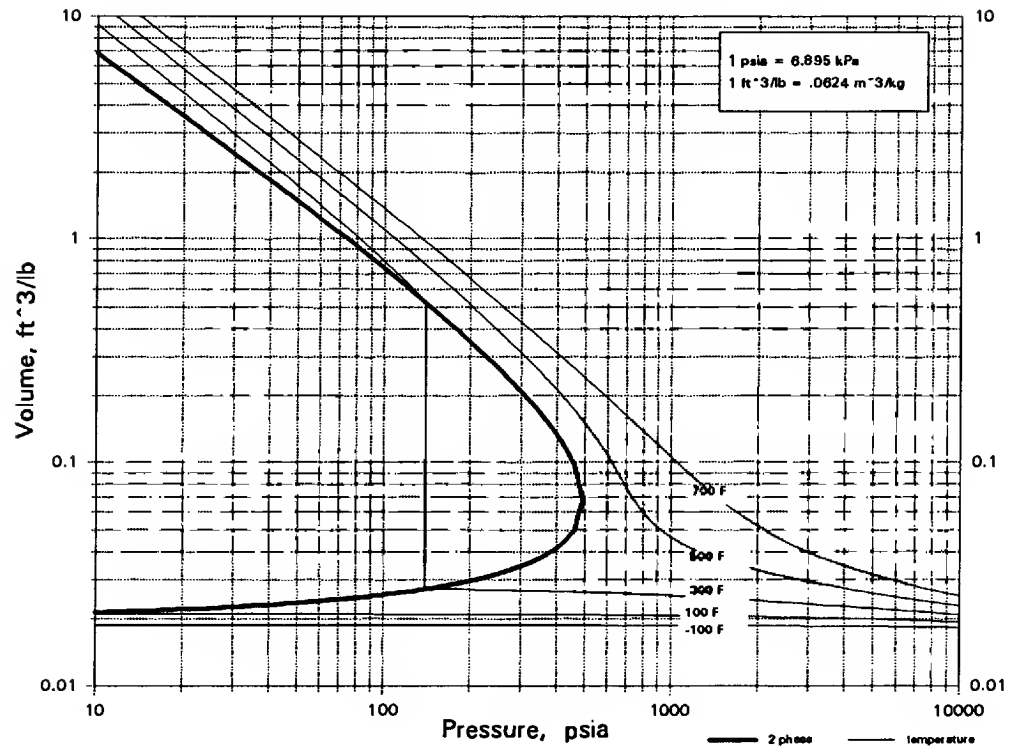
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METHYL tert-BUTYL ETHER



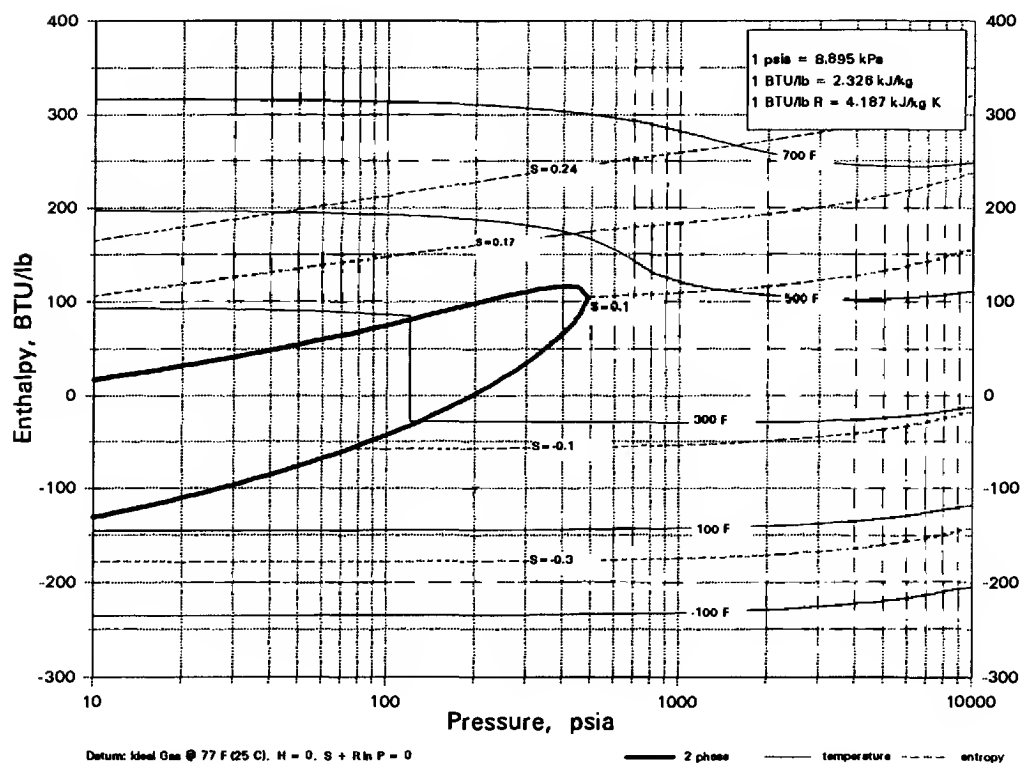
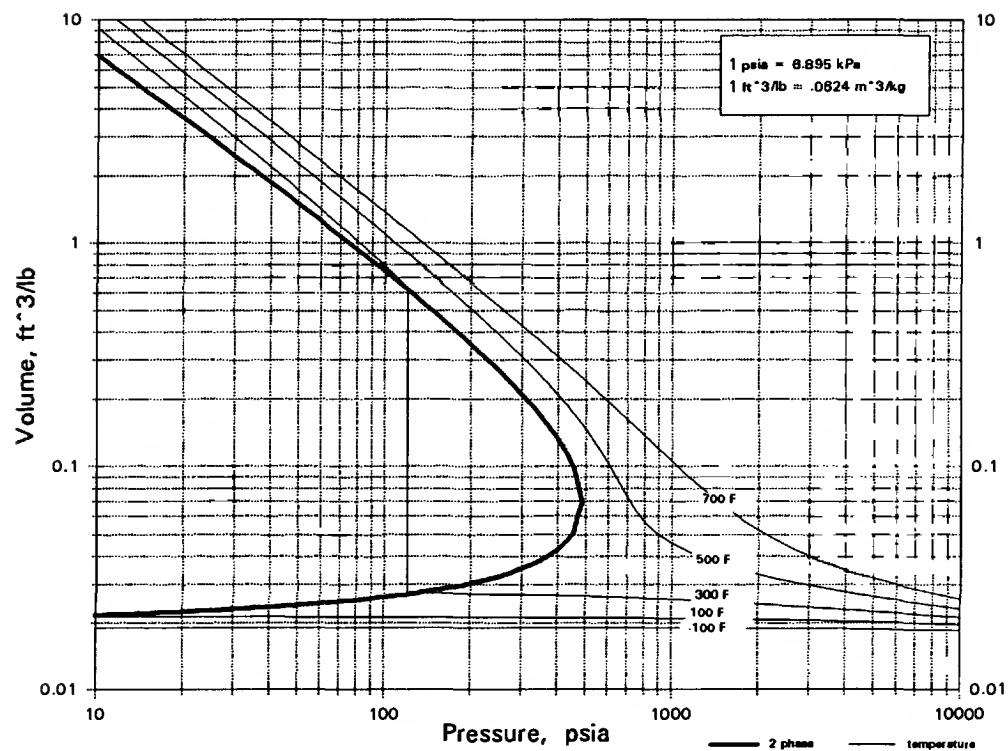
C5H12O

METHYL ISOBUTYL ETHER



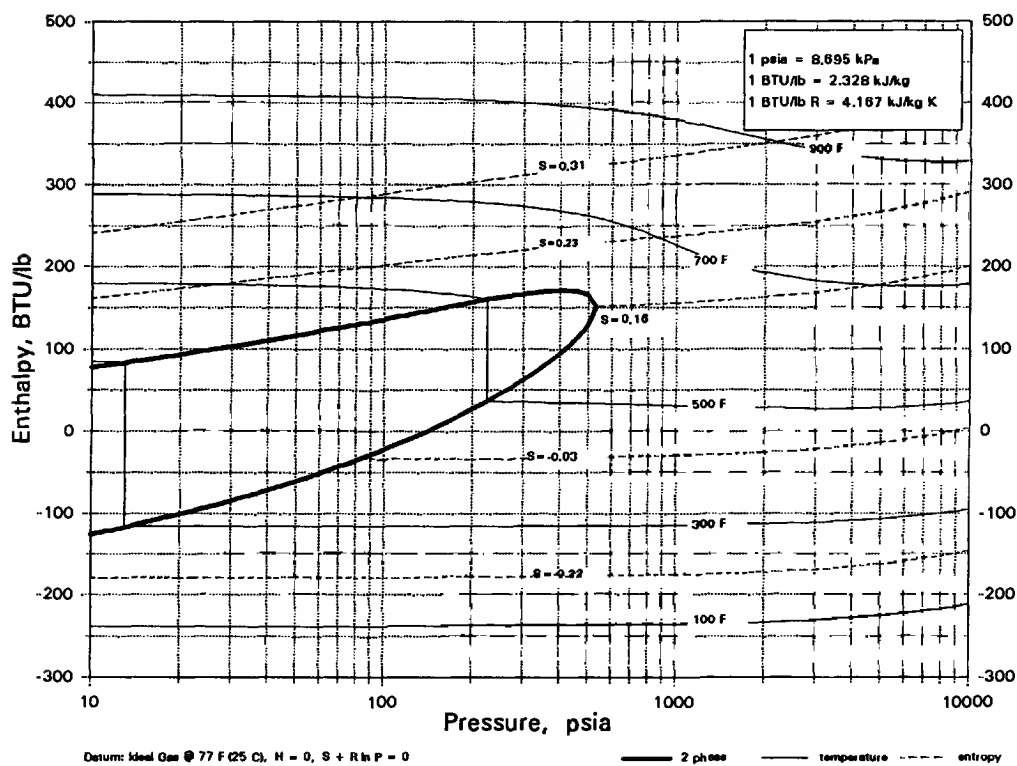
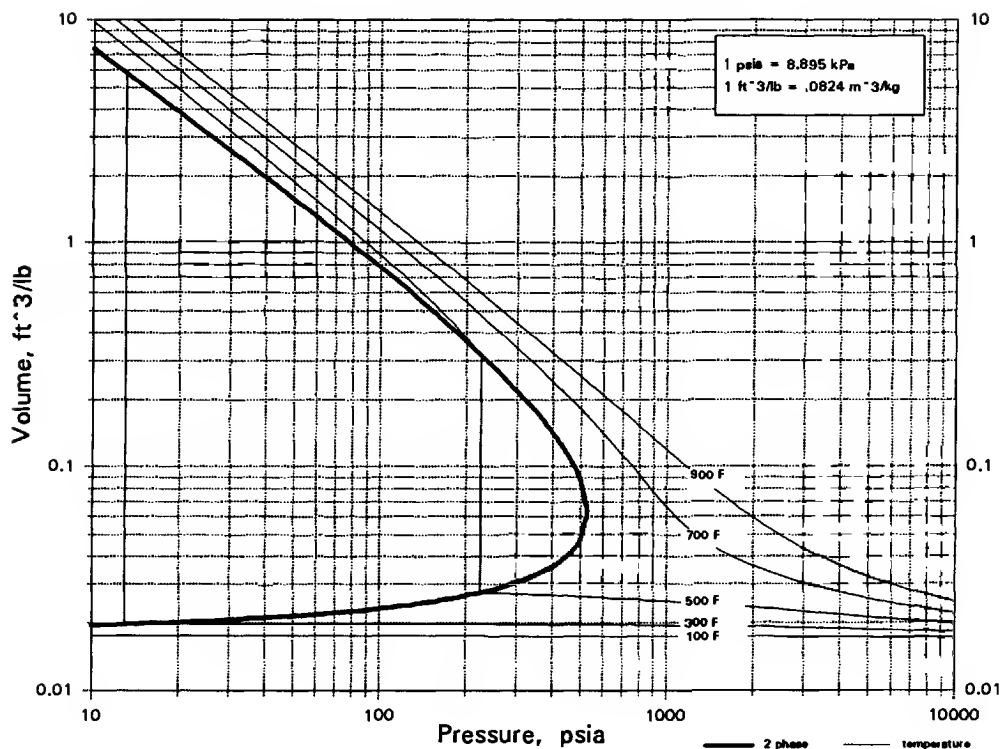
C5H12O

ETHYL PROPYL ETHER



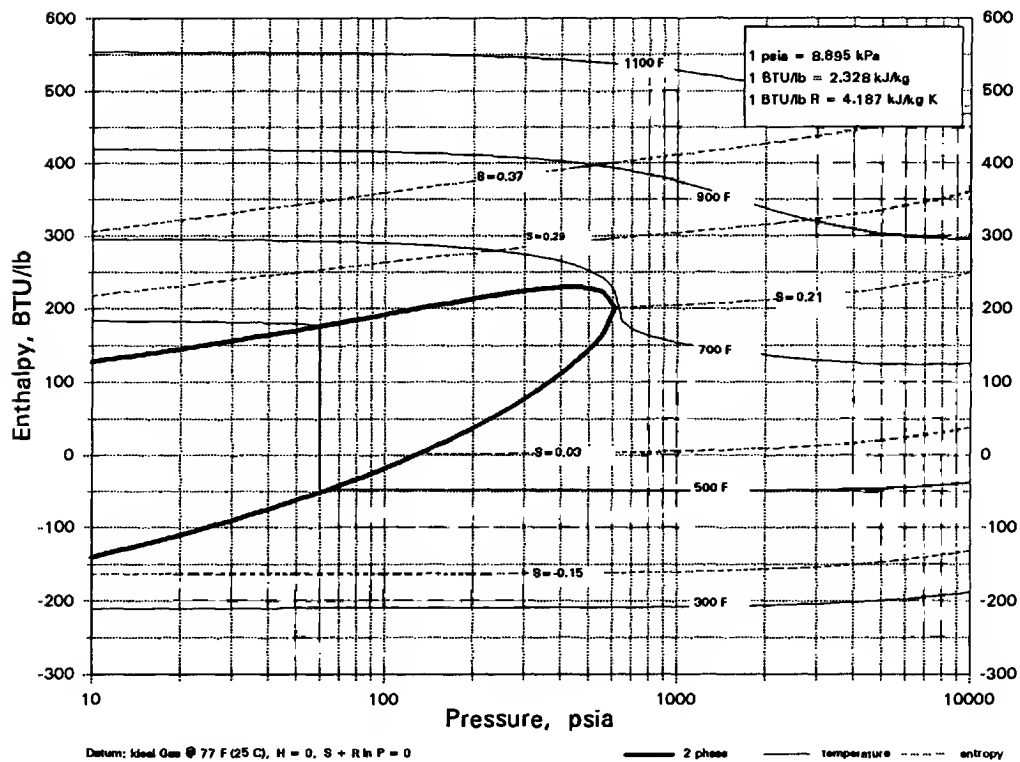
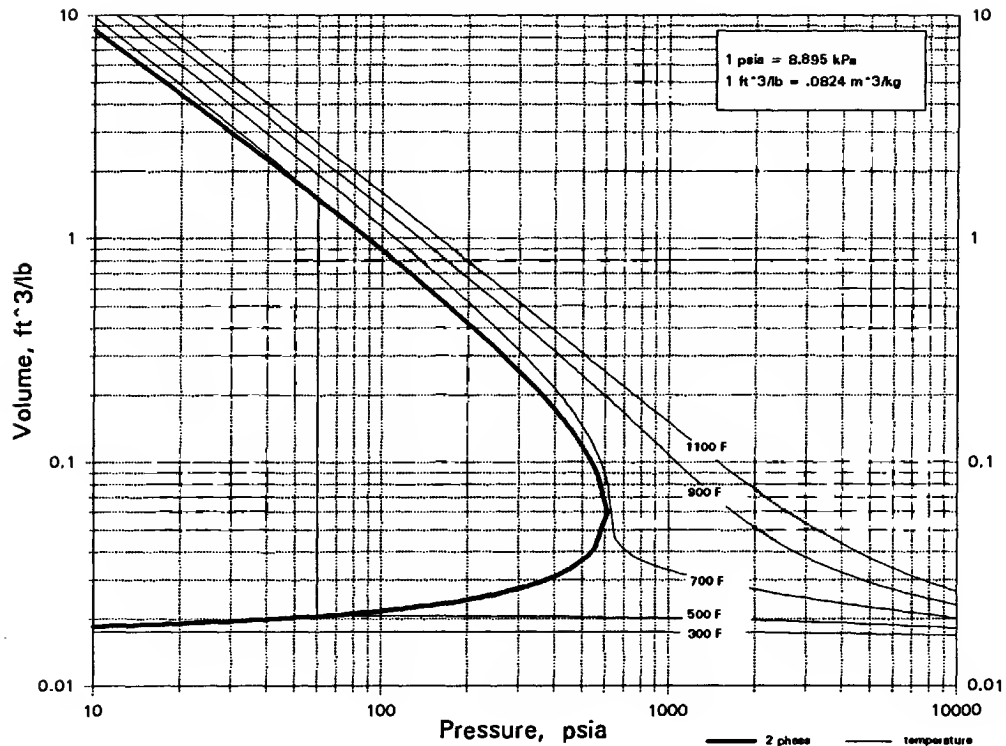
C5H12O2

ETHYLENE GLYCOL MONOPROPYL ETHER



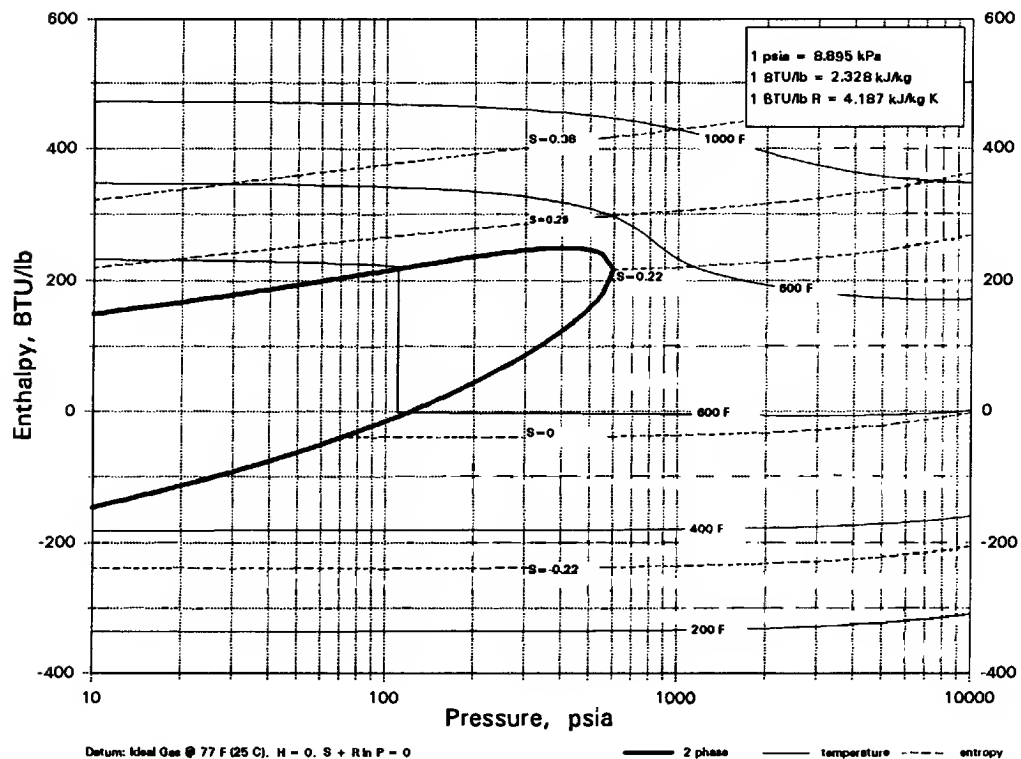
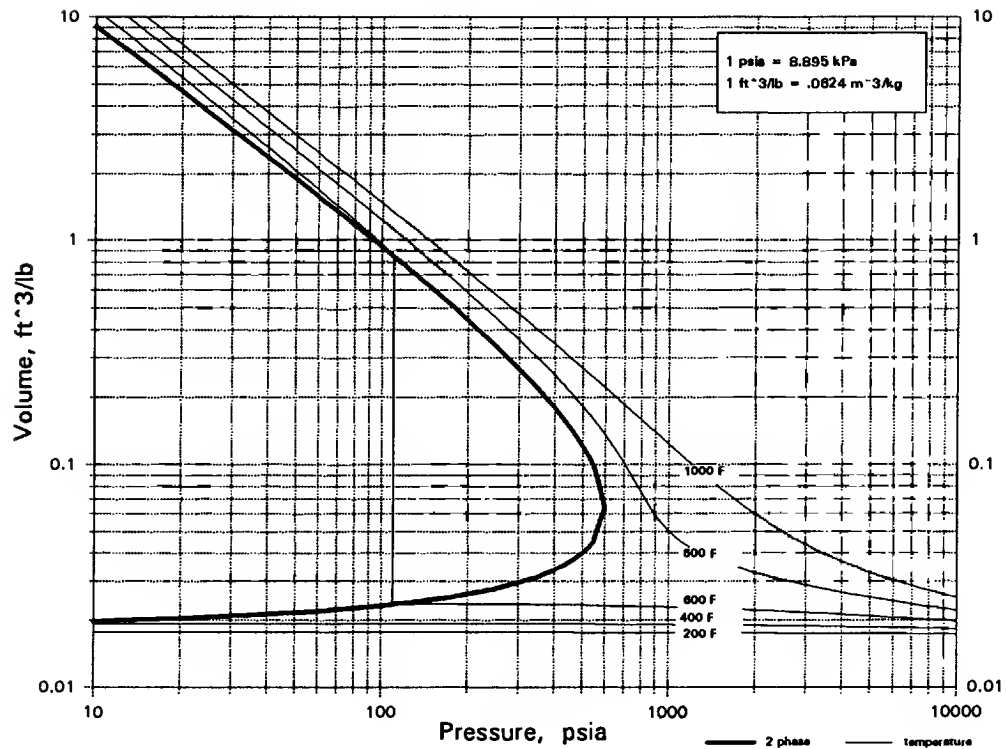
C5H12O2

NEOPENTYL GLYCOL



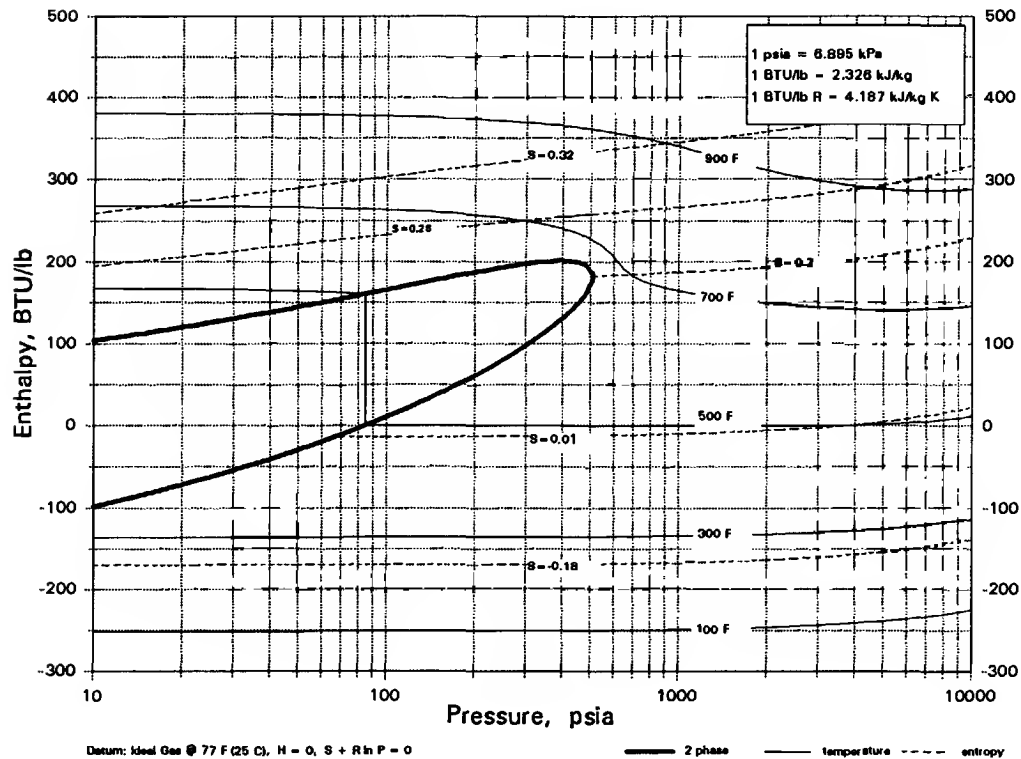
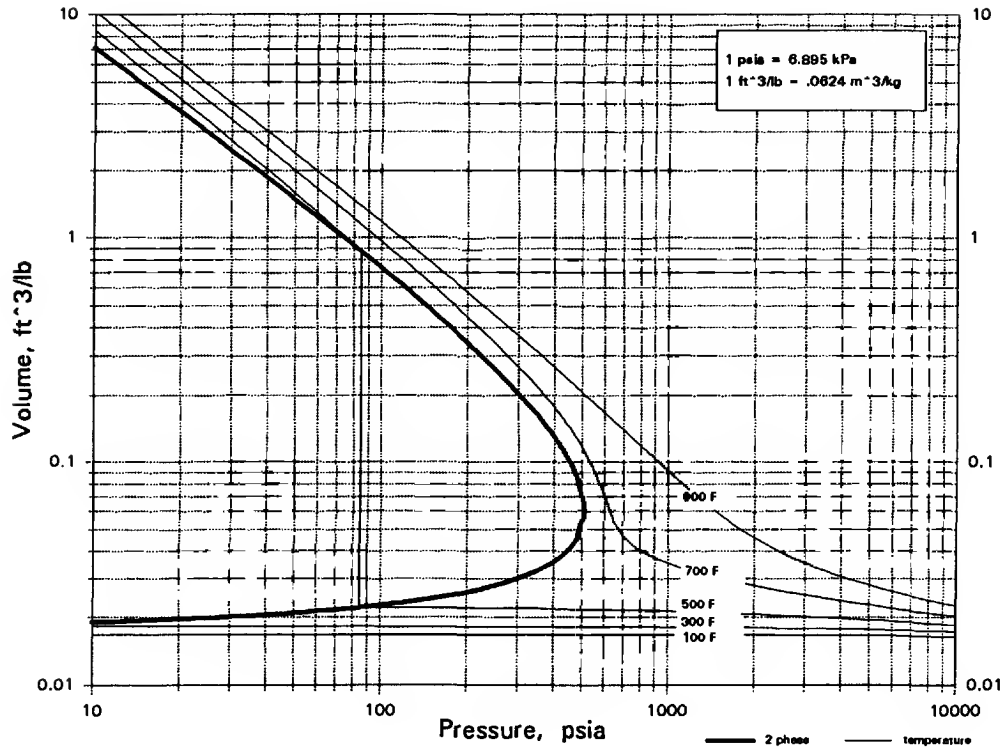
C5H12O2

1-5-PENTANEDIOL

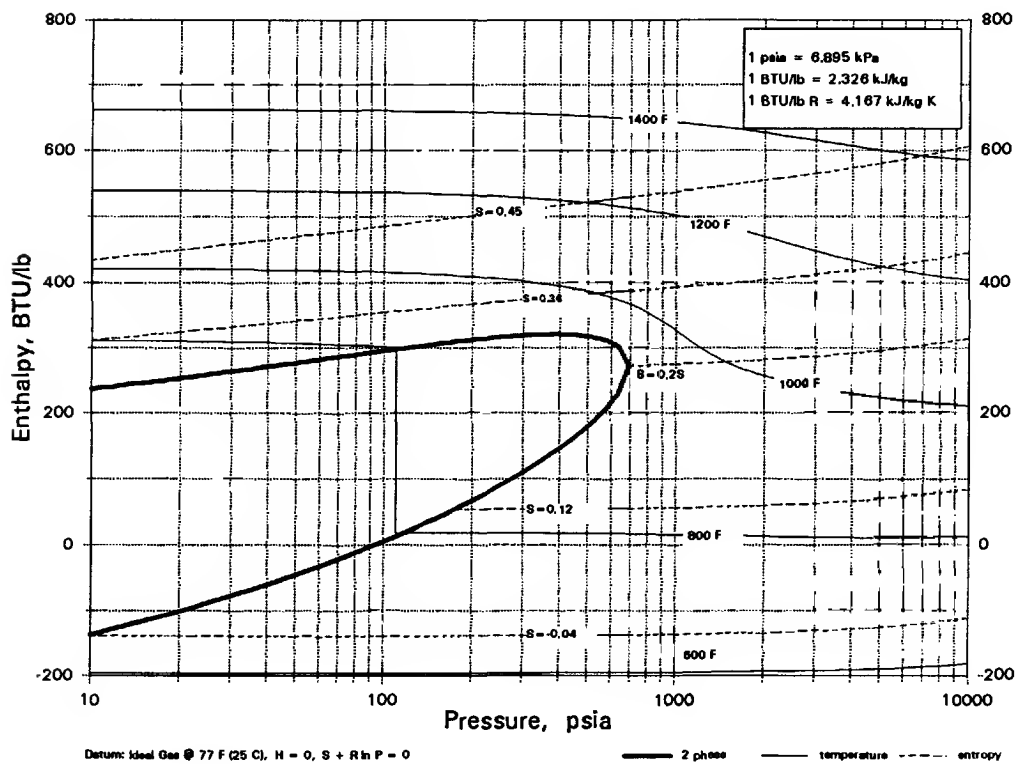
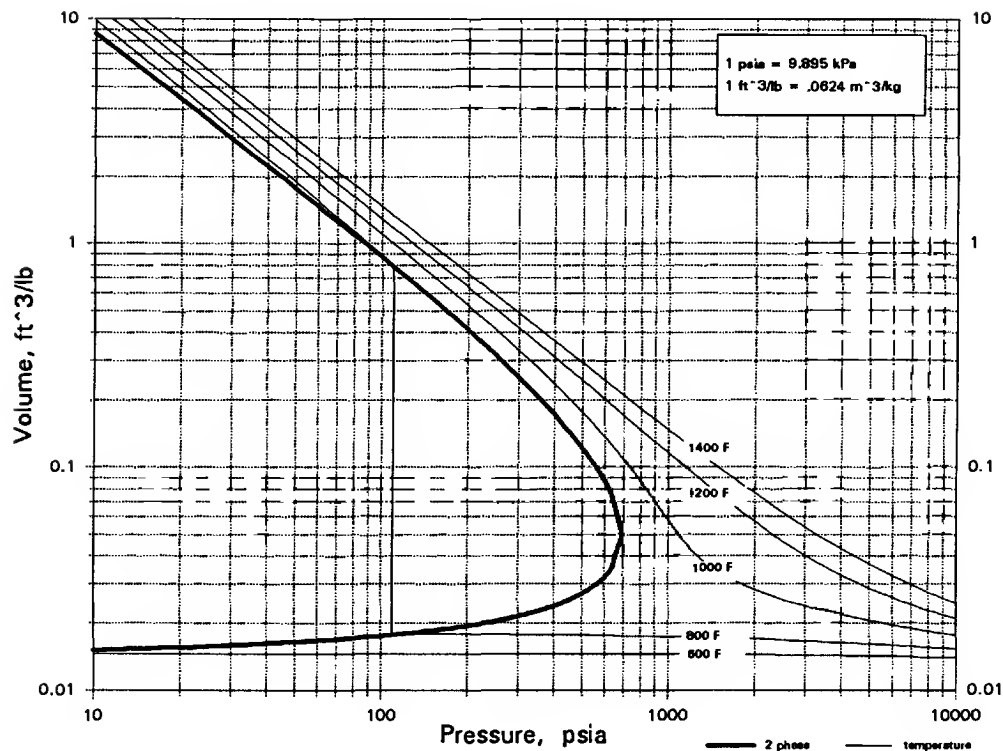


C5H12O3

2-(2-METHOXYETHOXY)ETHANOL

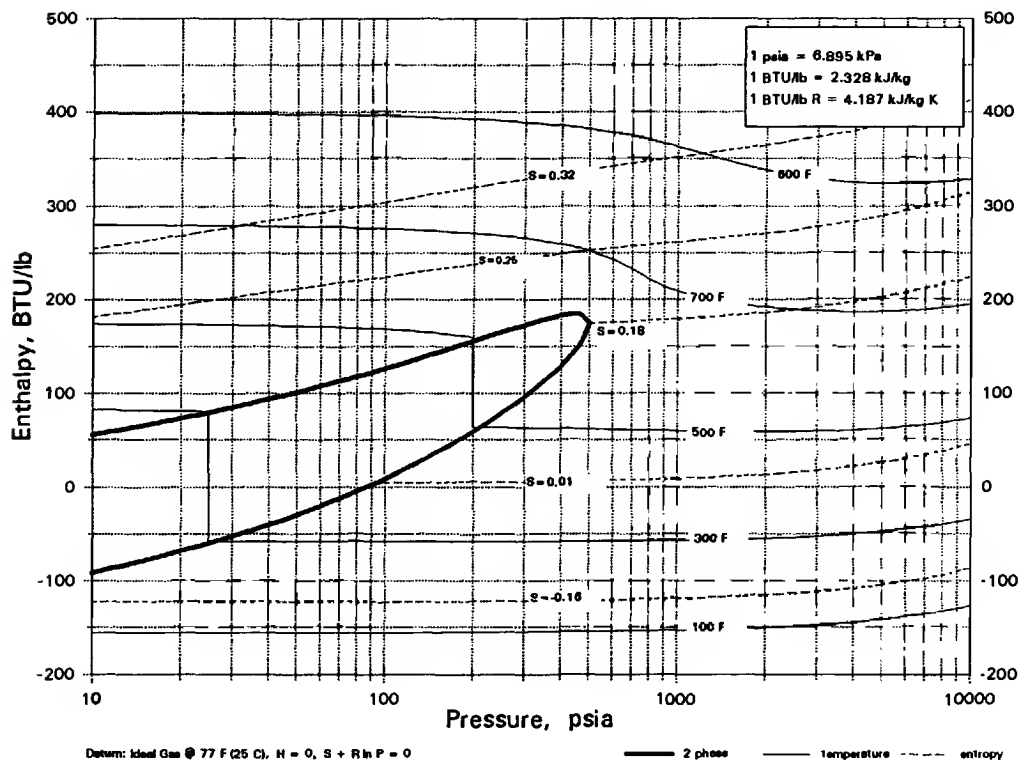
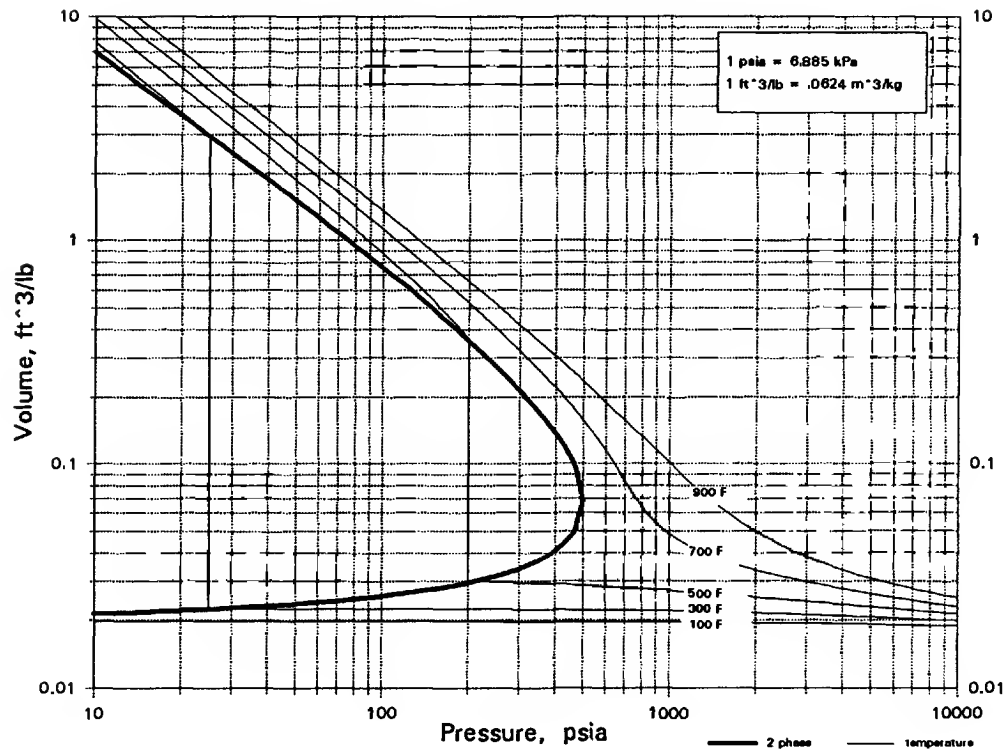


C5H12O4
PENTAERYTHRITOL



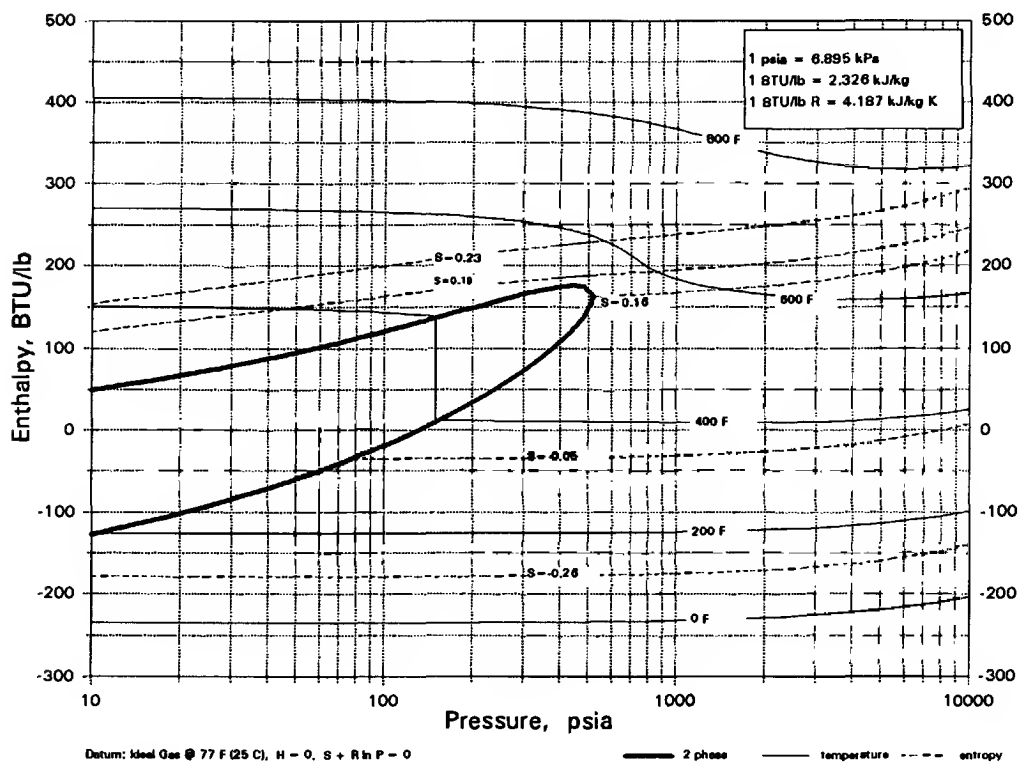
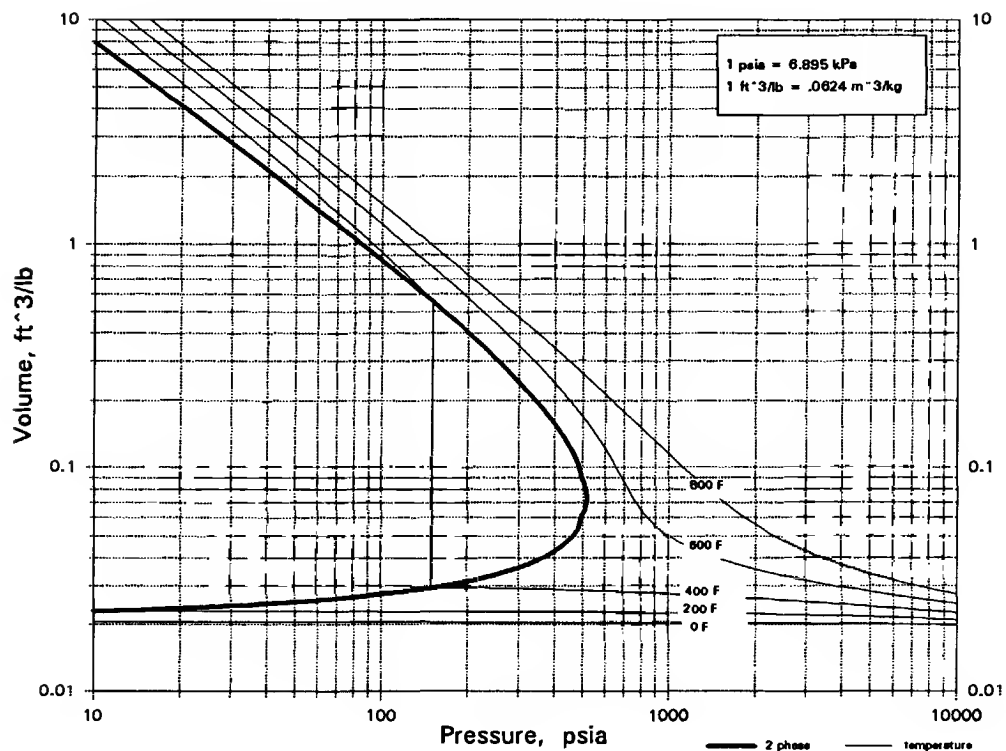
C5H12S

n-PENTYL MERCAPTAN



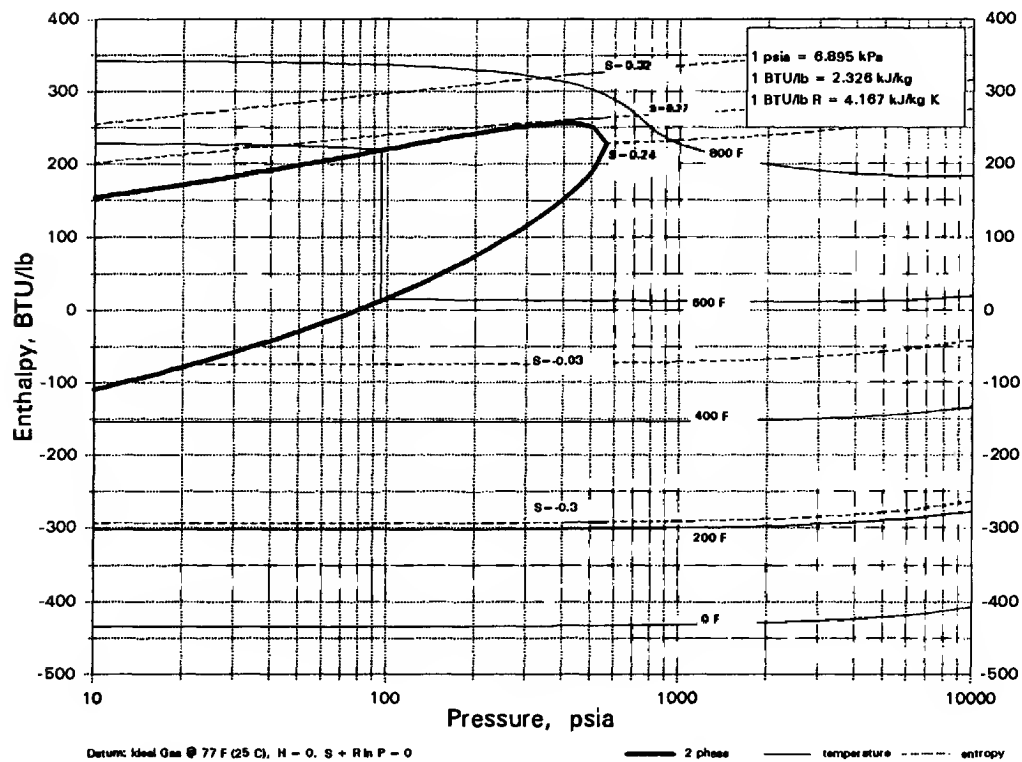
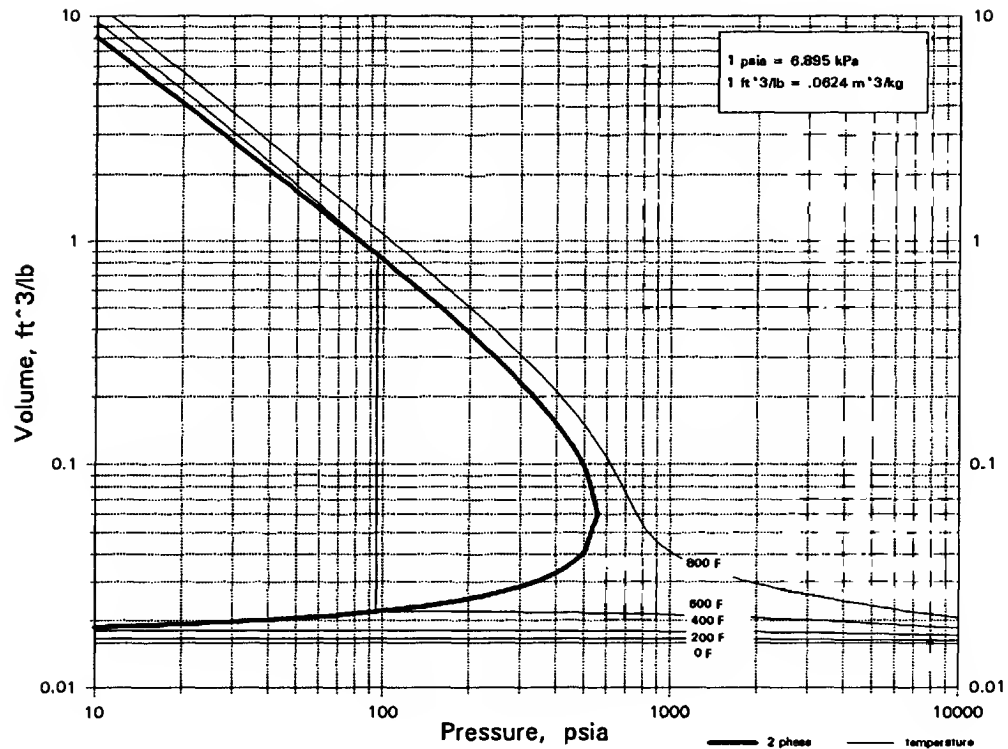
C5H13N

n-PENTYLAMINE

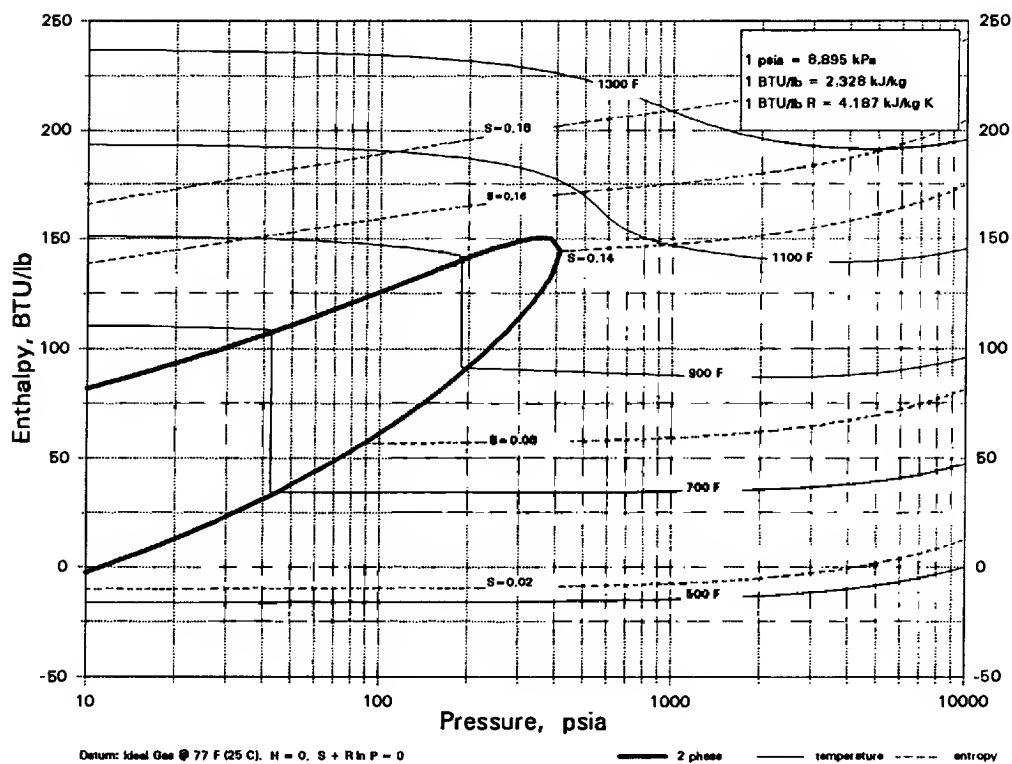
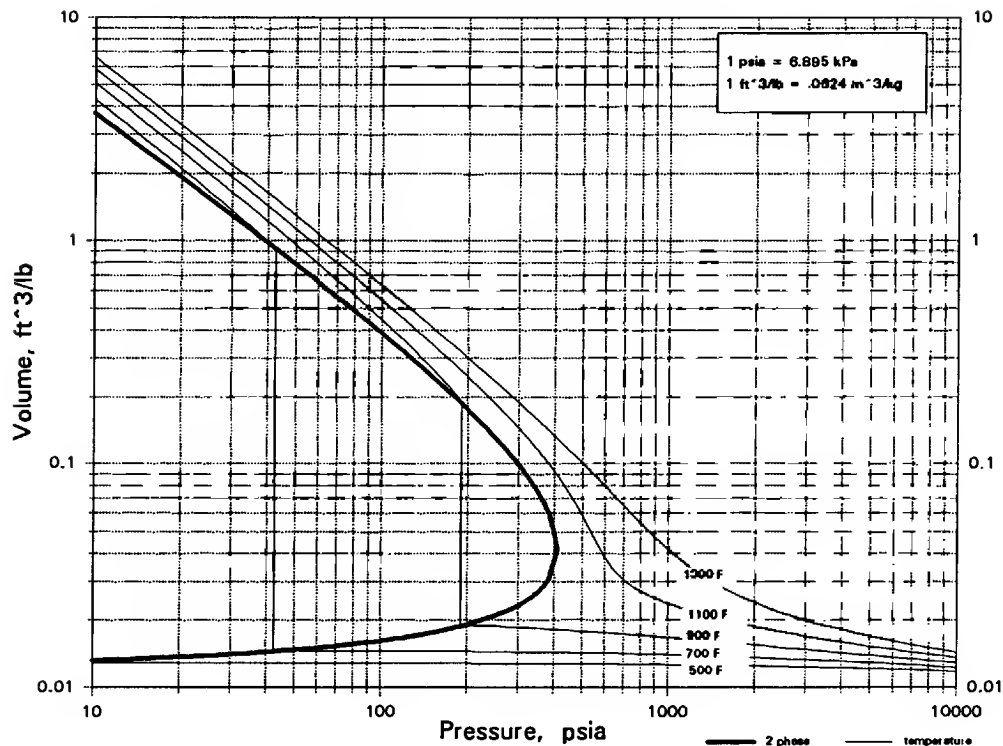


C5H13NO2

METHYL DIETHANOLAMINE

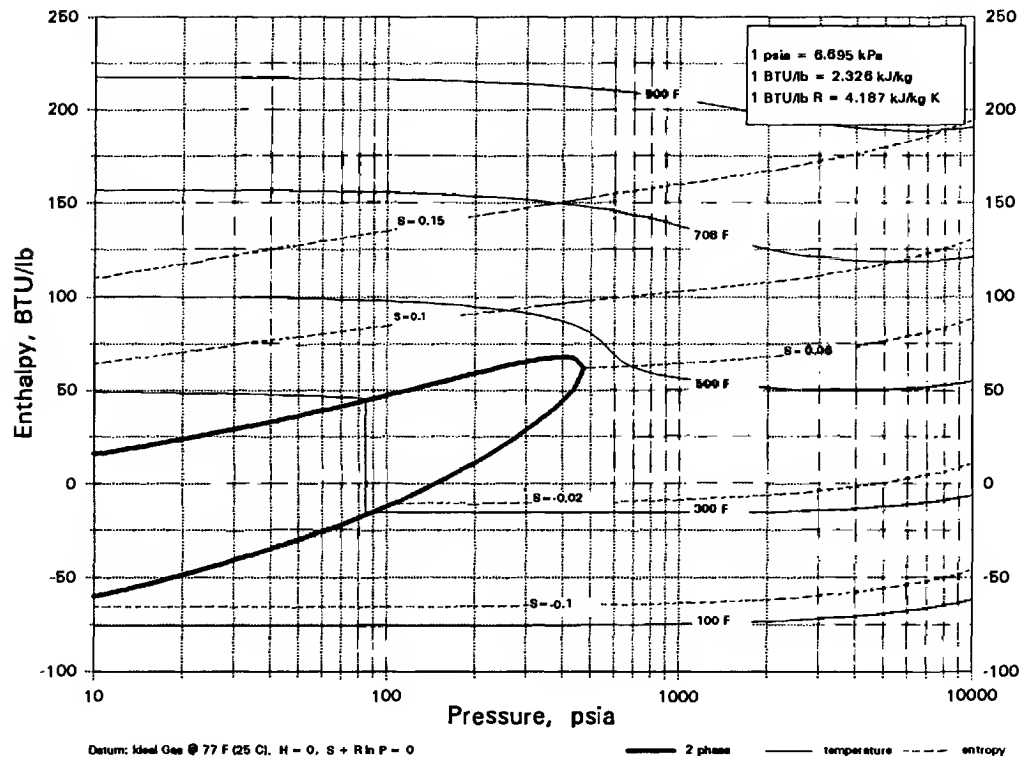
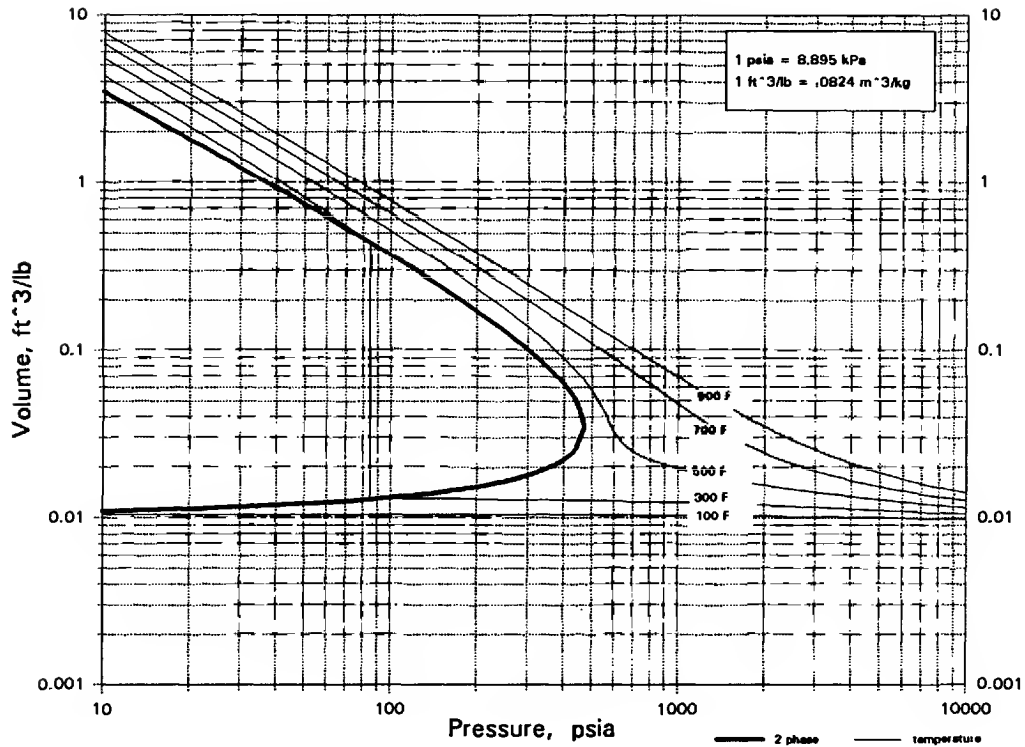


C6Cl6
HEXACHLOROBENZENE

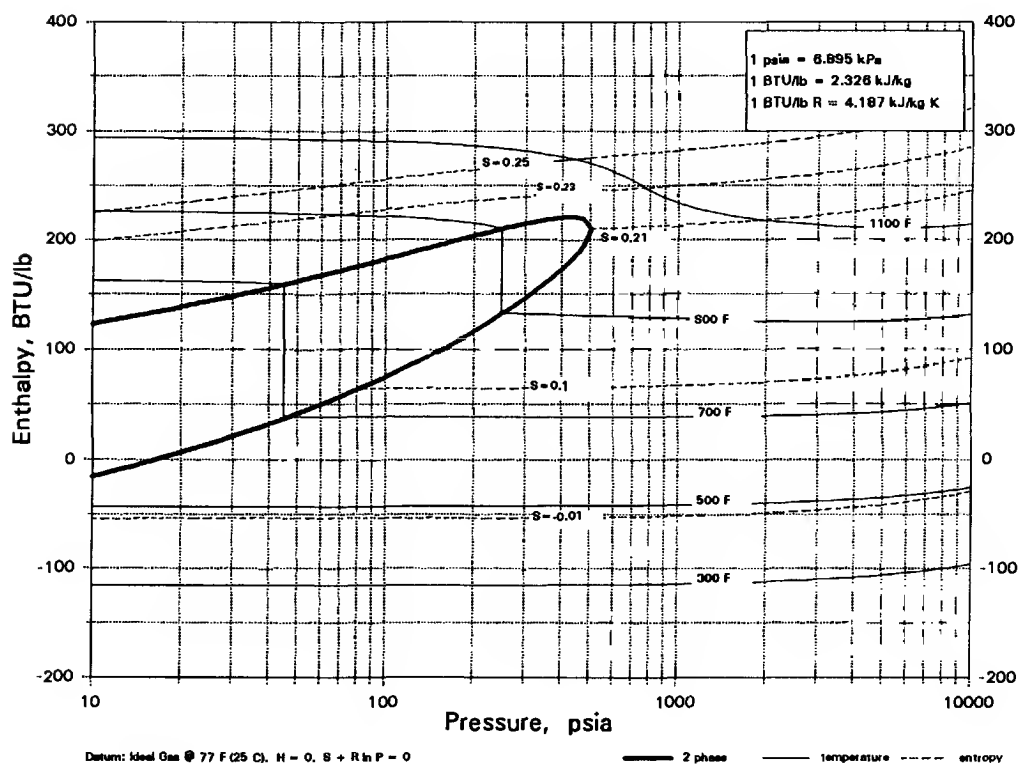
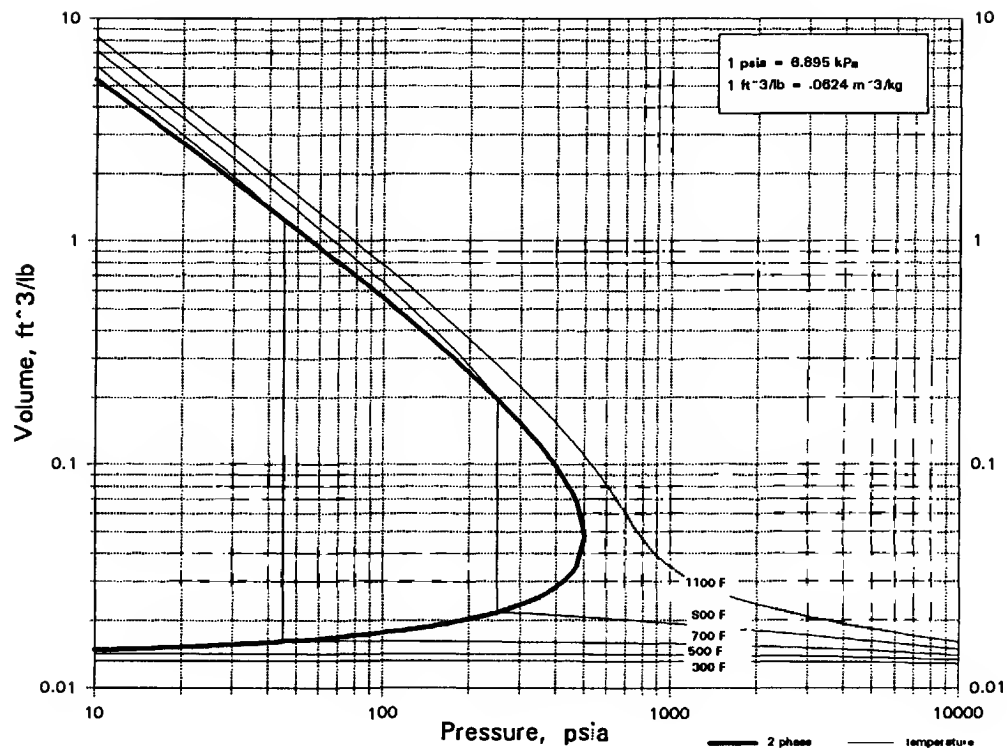


C6F6

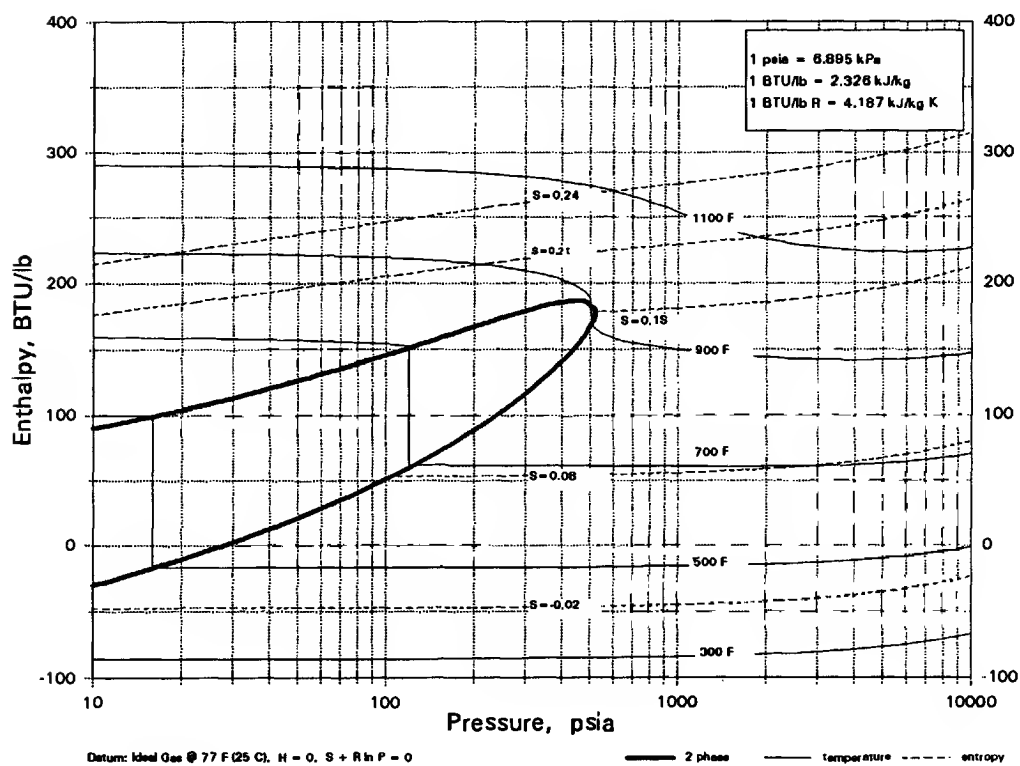
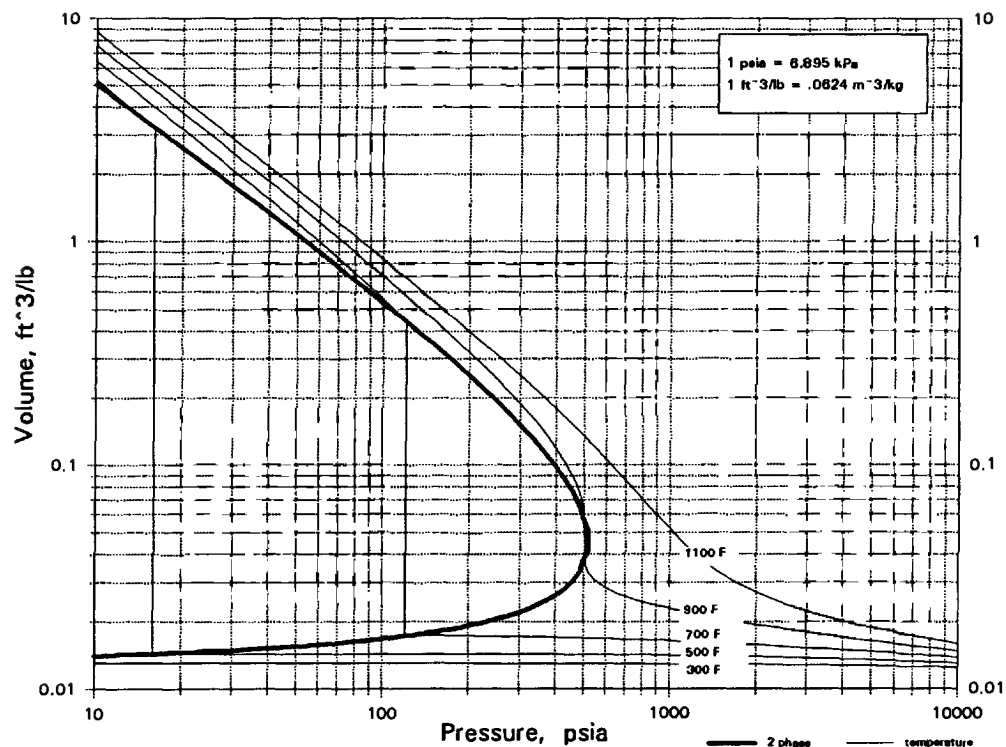
HEXAFLUOROBENZENE



C6H3ClN2O4 1-CHLORO-2,4-DINITROBENZENE

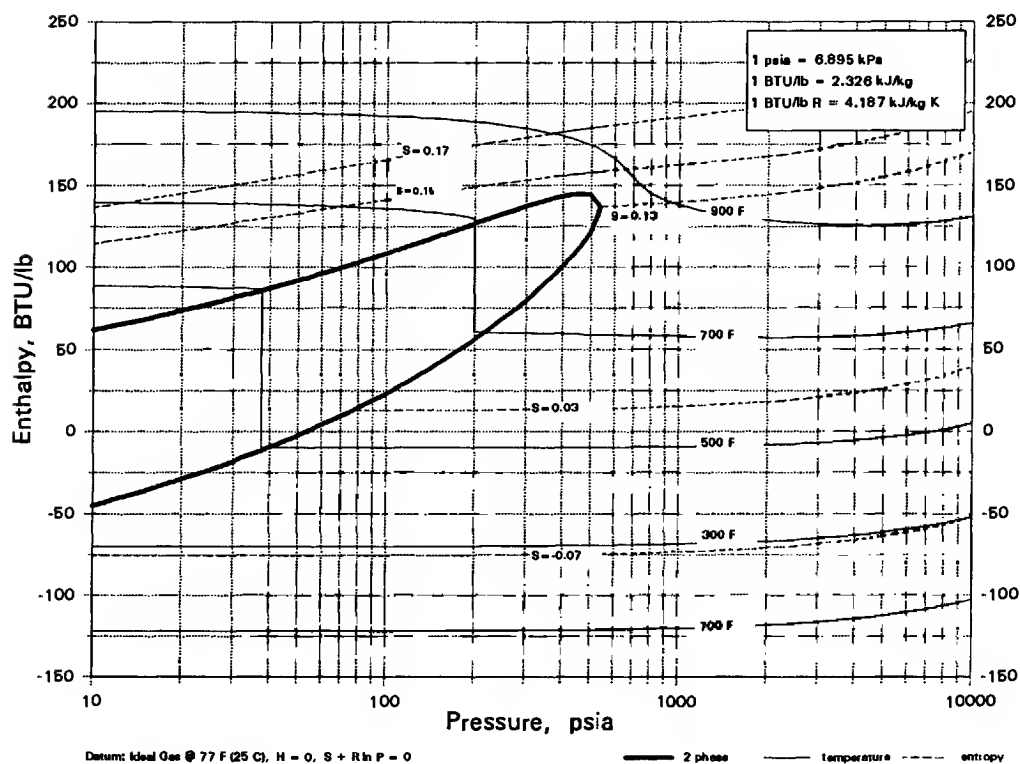
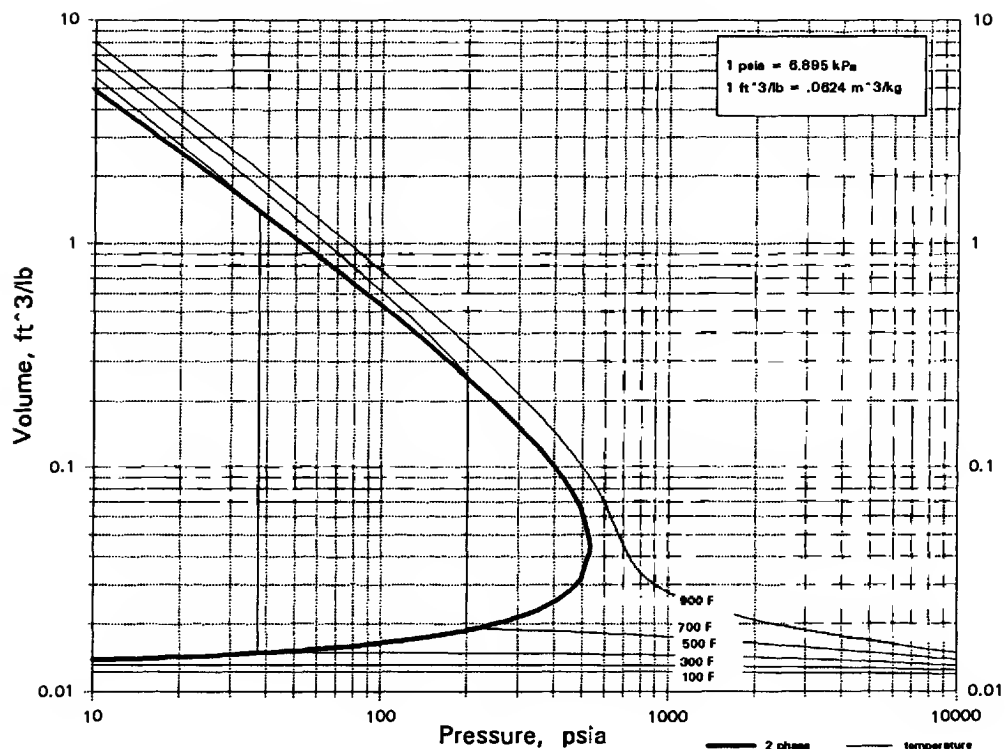


C6H3Cl2NO2 1-2-DICHLORO-4-NITROBENZENE



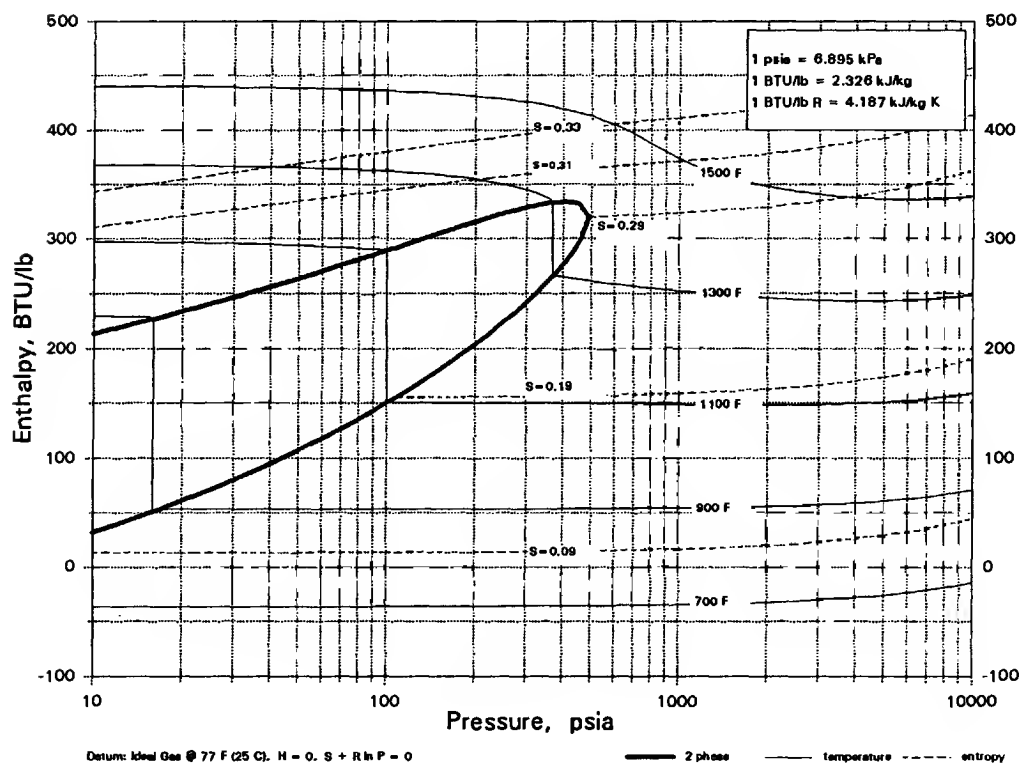
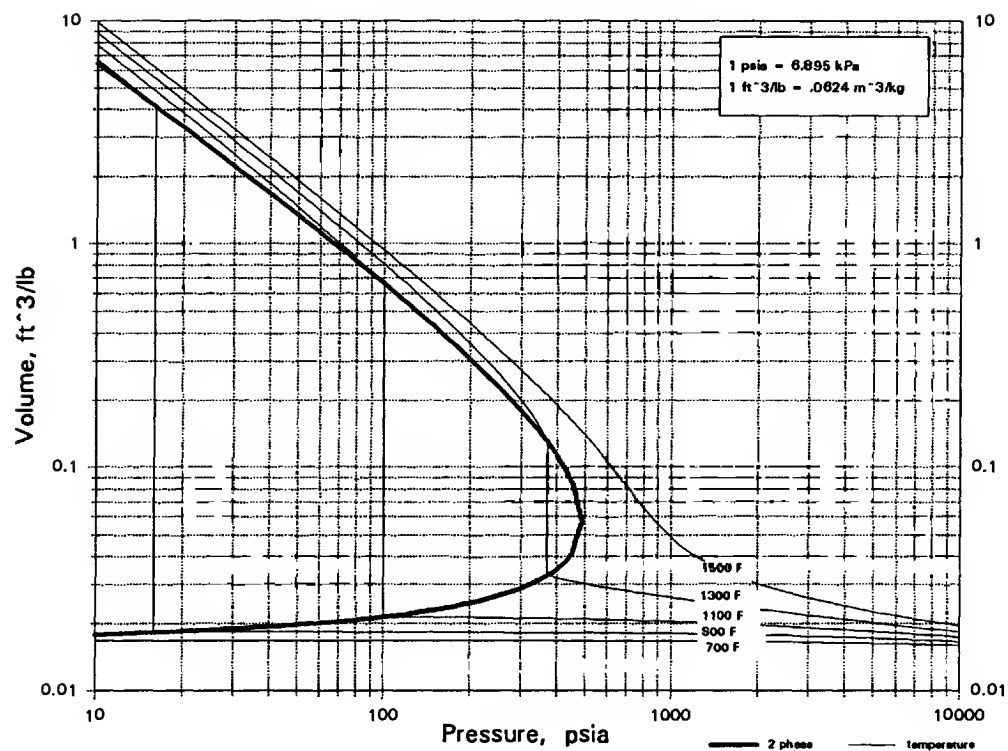
C6H3Cl3

1-2-4-TRICHLOROBENZENE



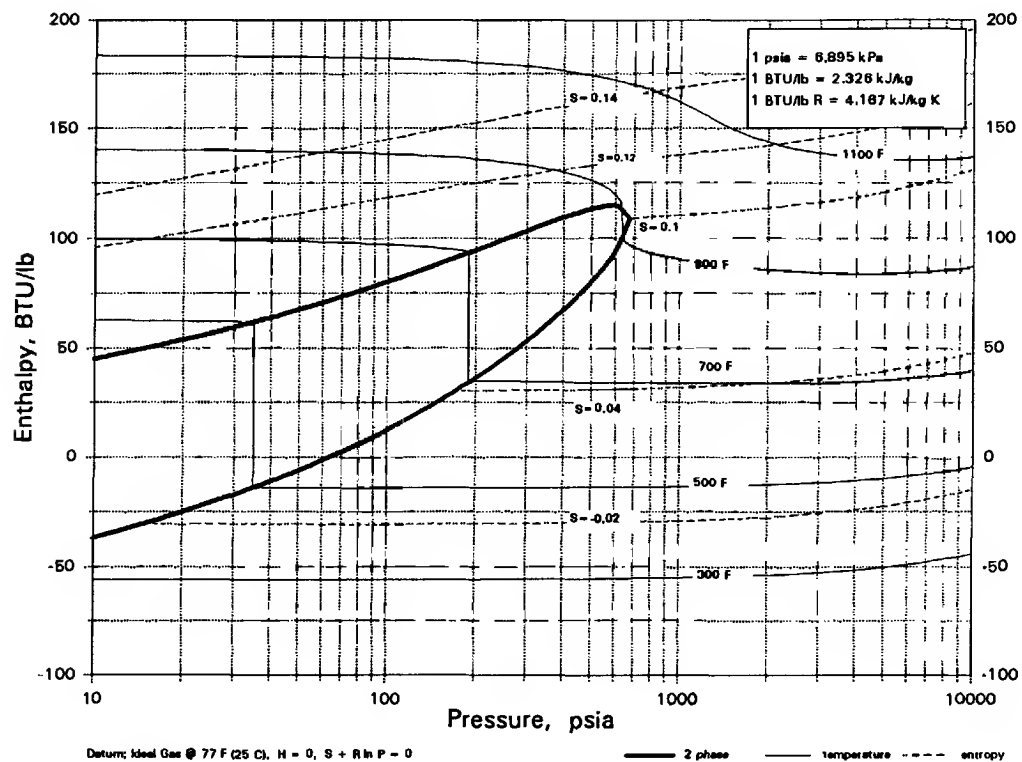
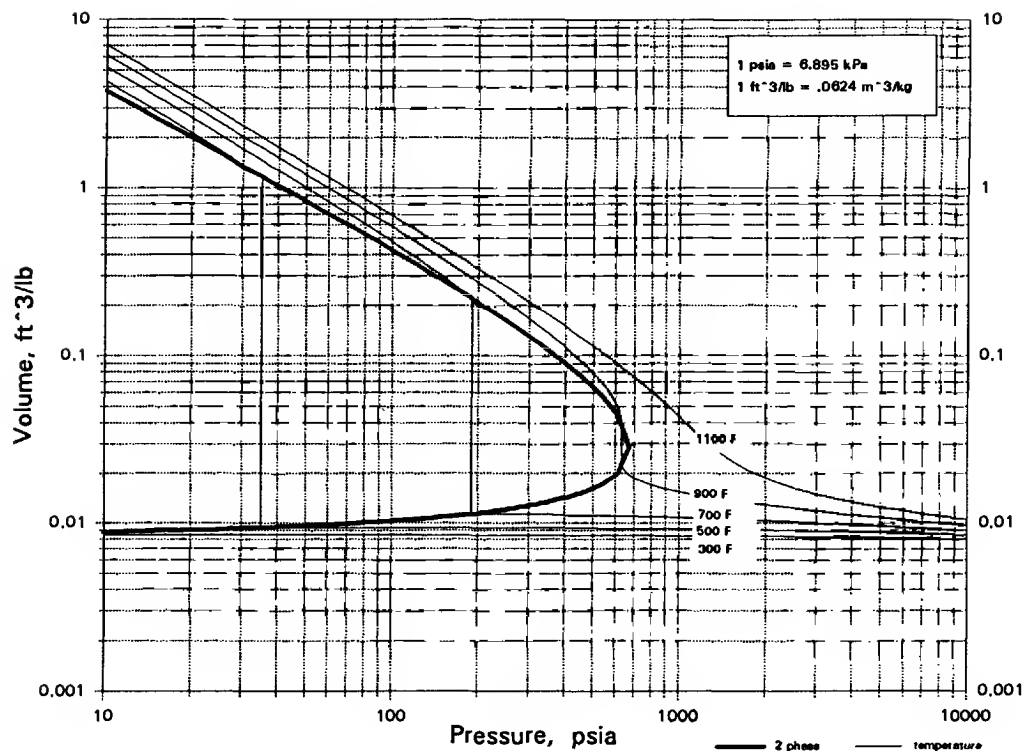
C6H3N3O6

1-3-5-TRINITROBENZENE

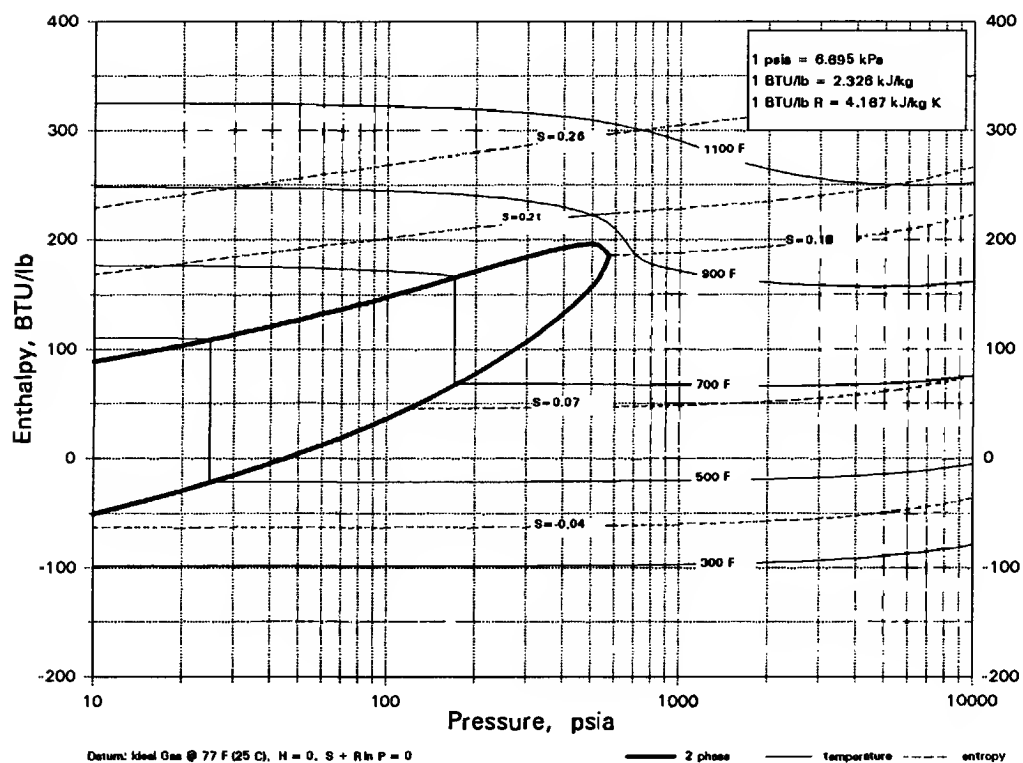
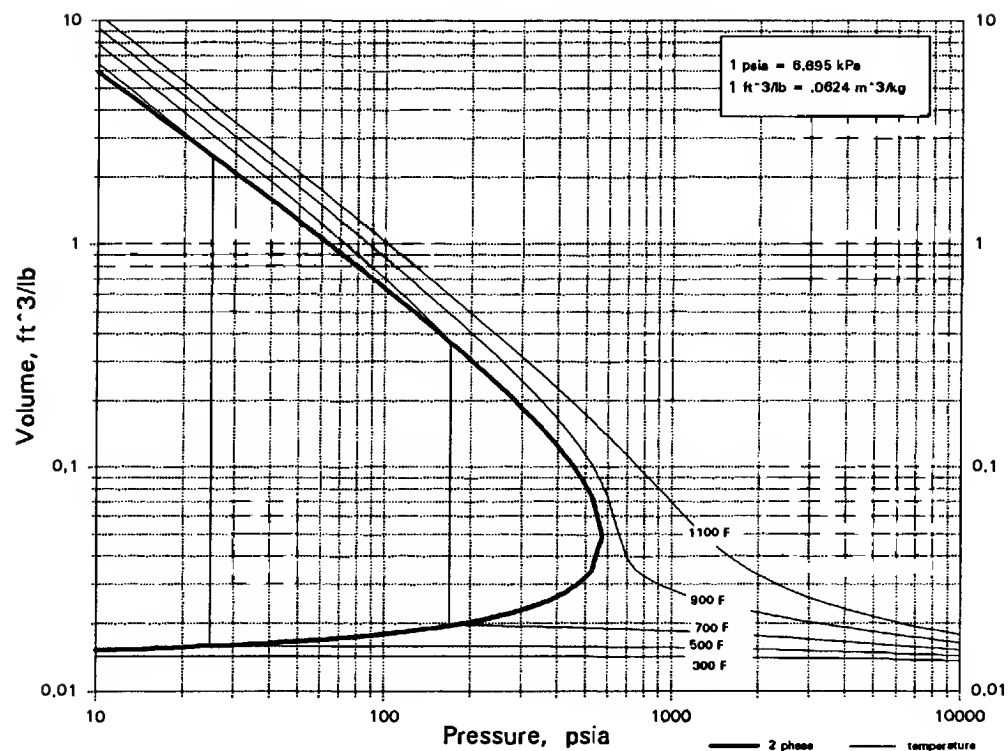


C6H4Br2

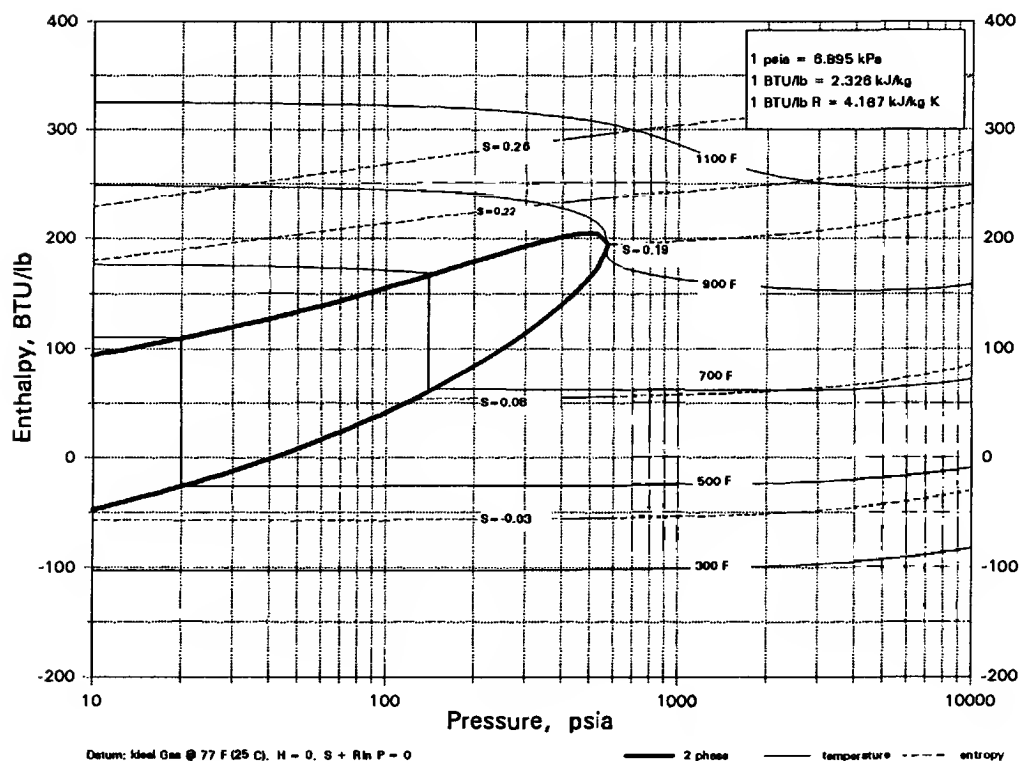
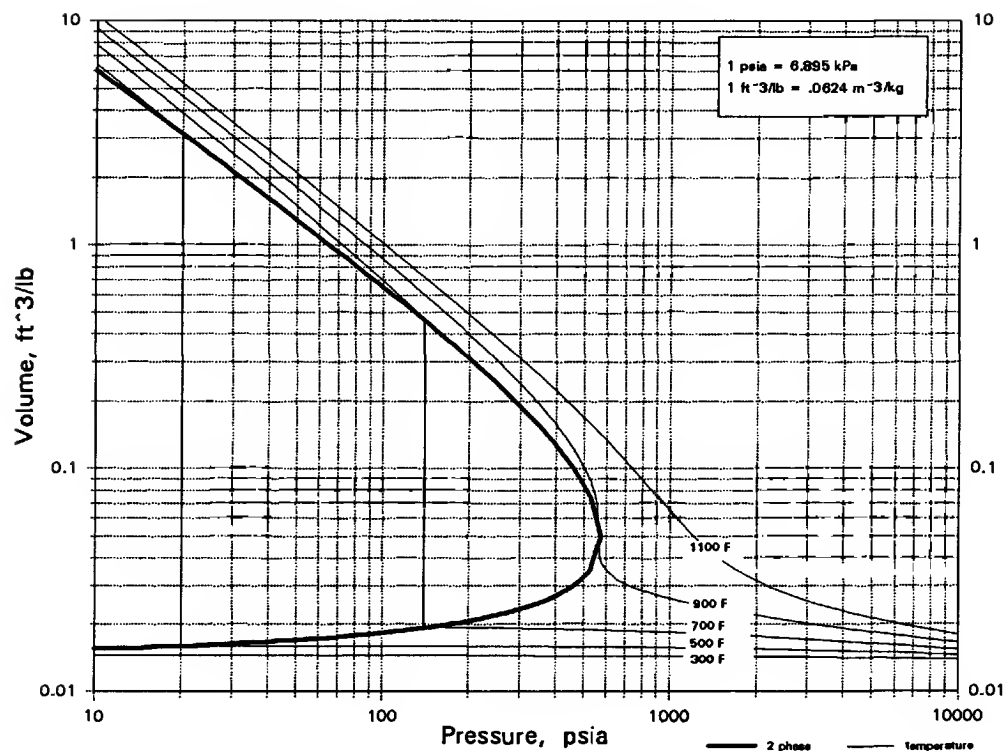
m-DIBROMOBENZENE



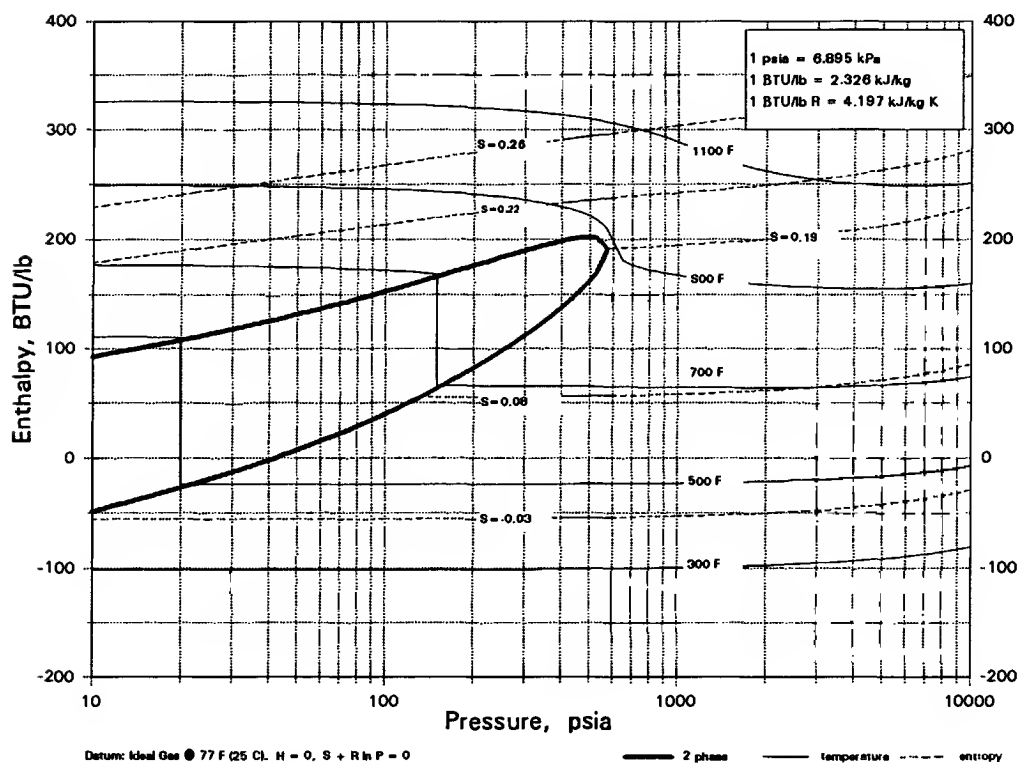
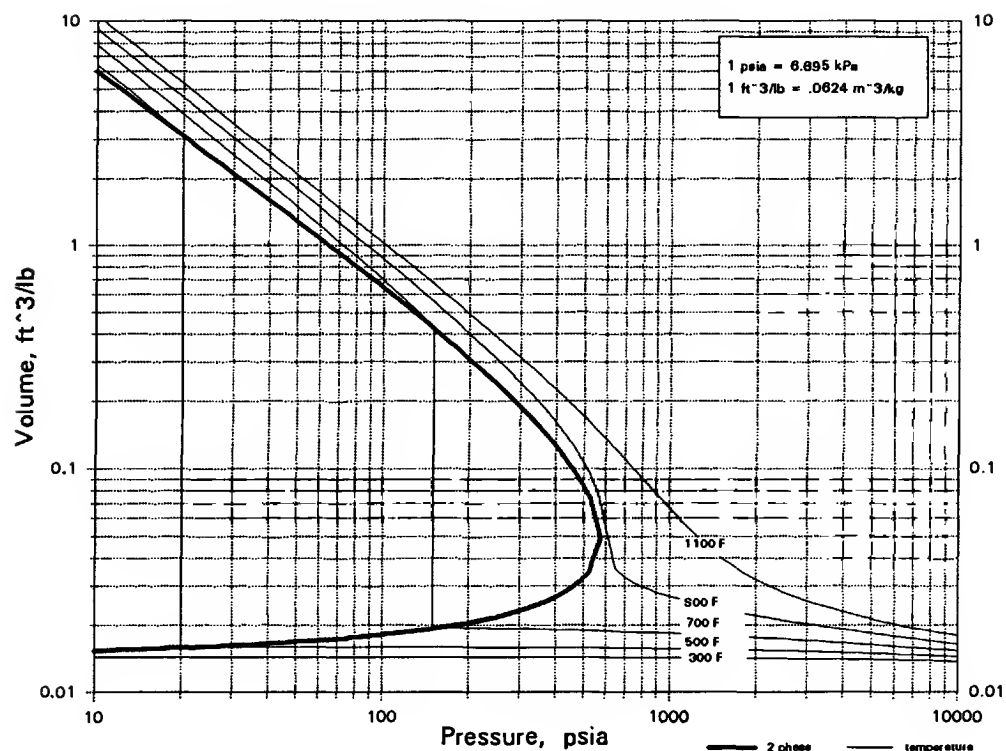
C₆H₄ClNO₂ m-CHLORONITROBENZENE



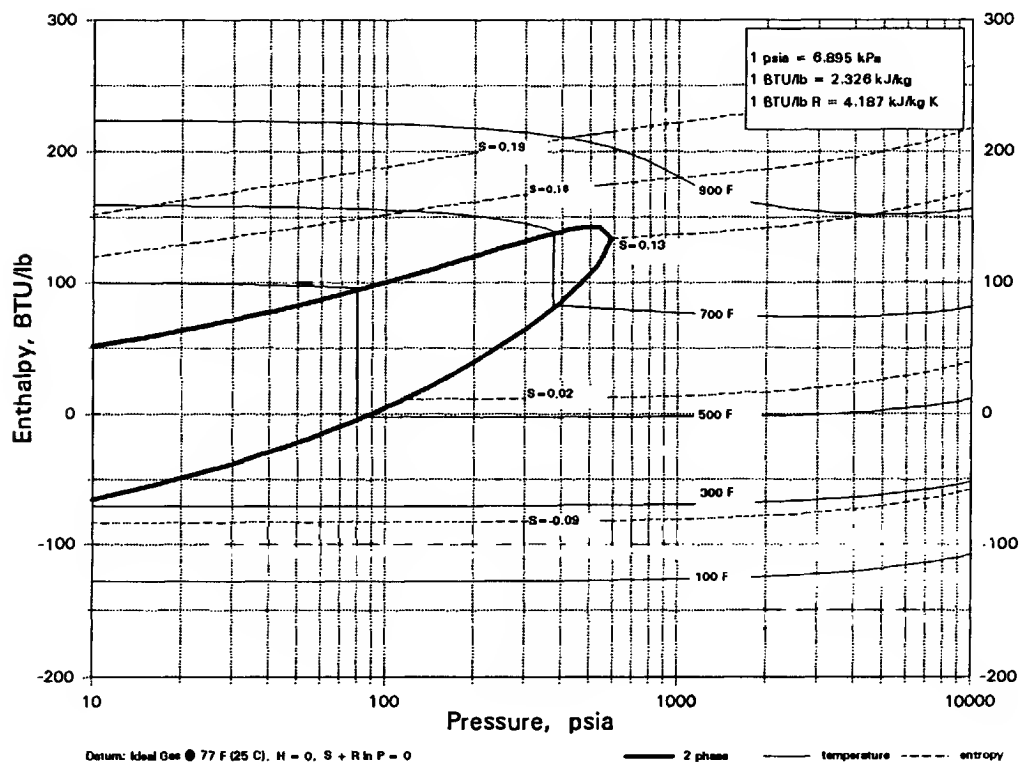
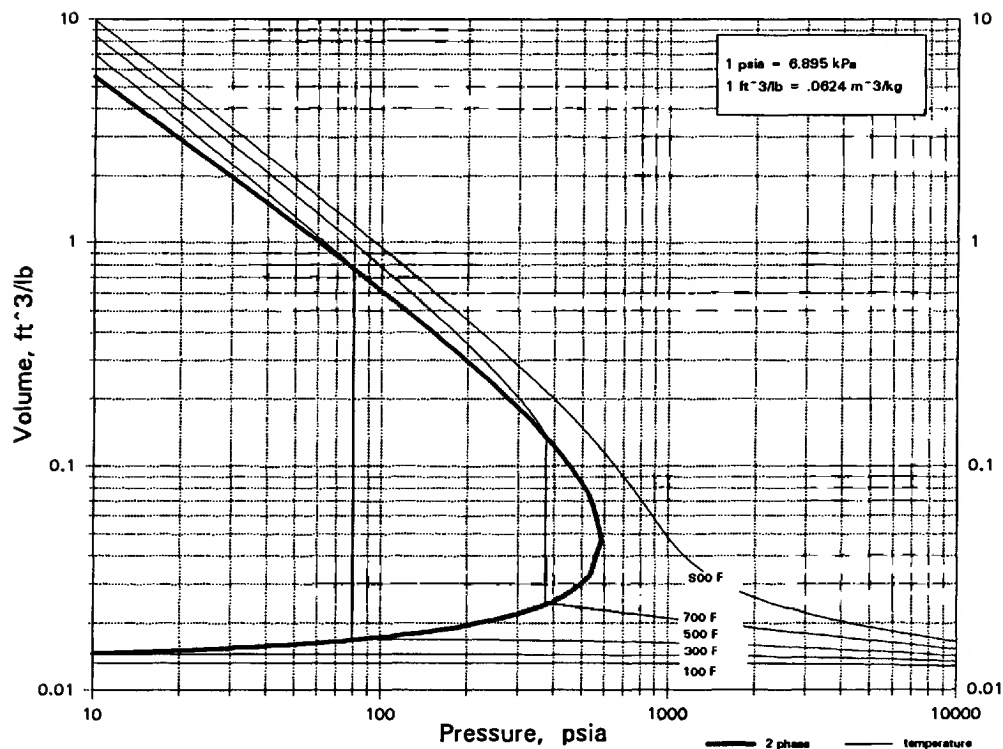
C₆H₄ClNO₂ o-CHLORONITROBENZENE



C6H4ClNO2 p-CHLORONITROBENZENE

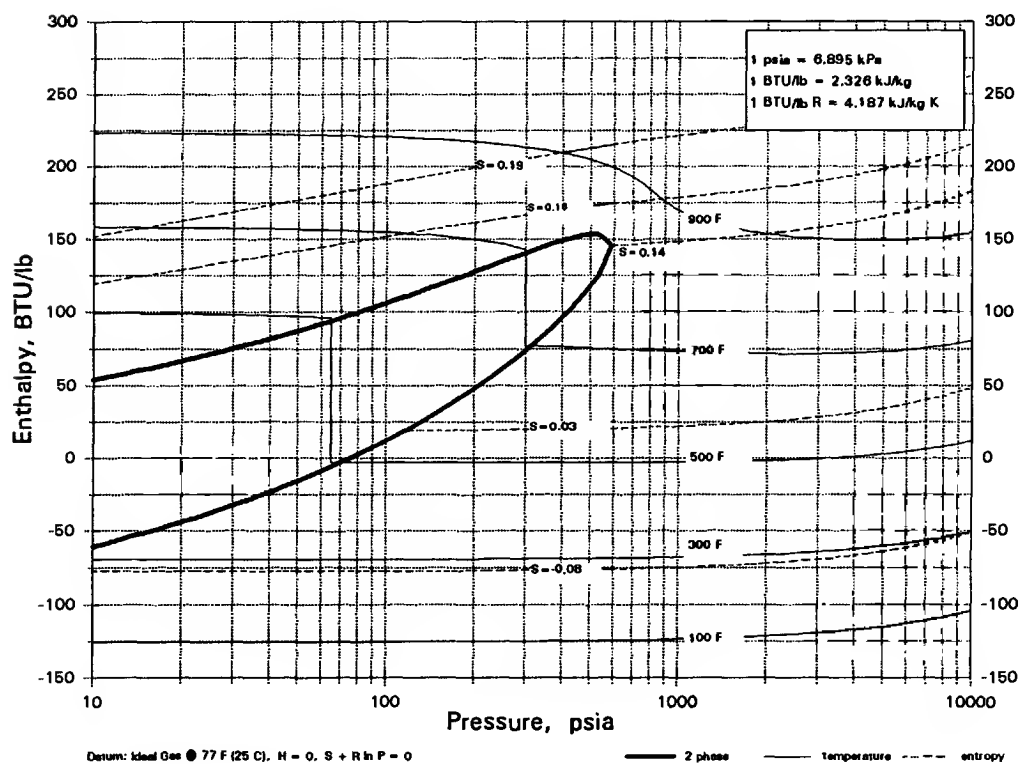
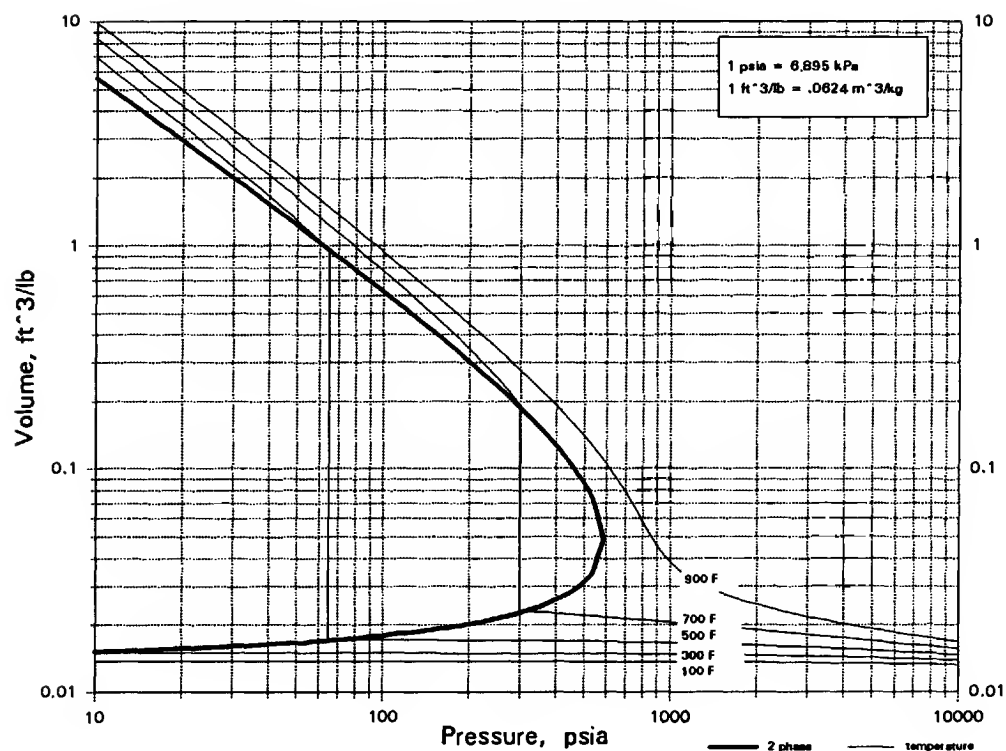


C₆H₄Cl₂
m-DICHLOROBENZENE



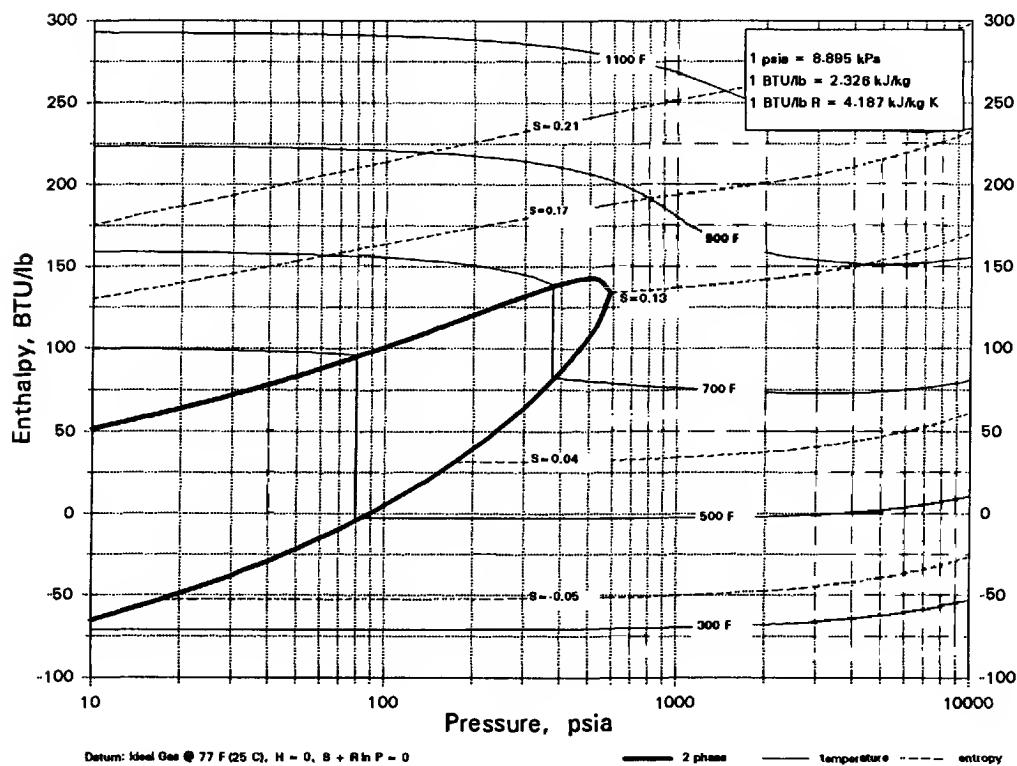
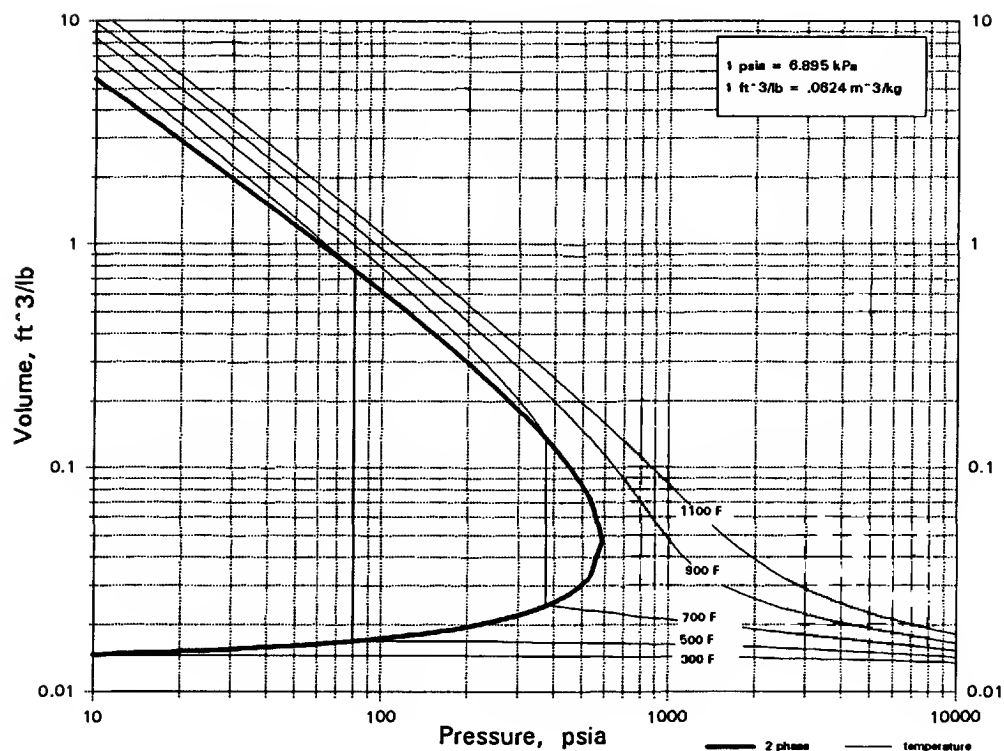
C6H4Cl2

o-DICHLOROBENZENE



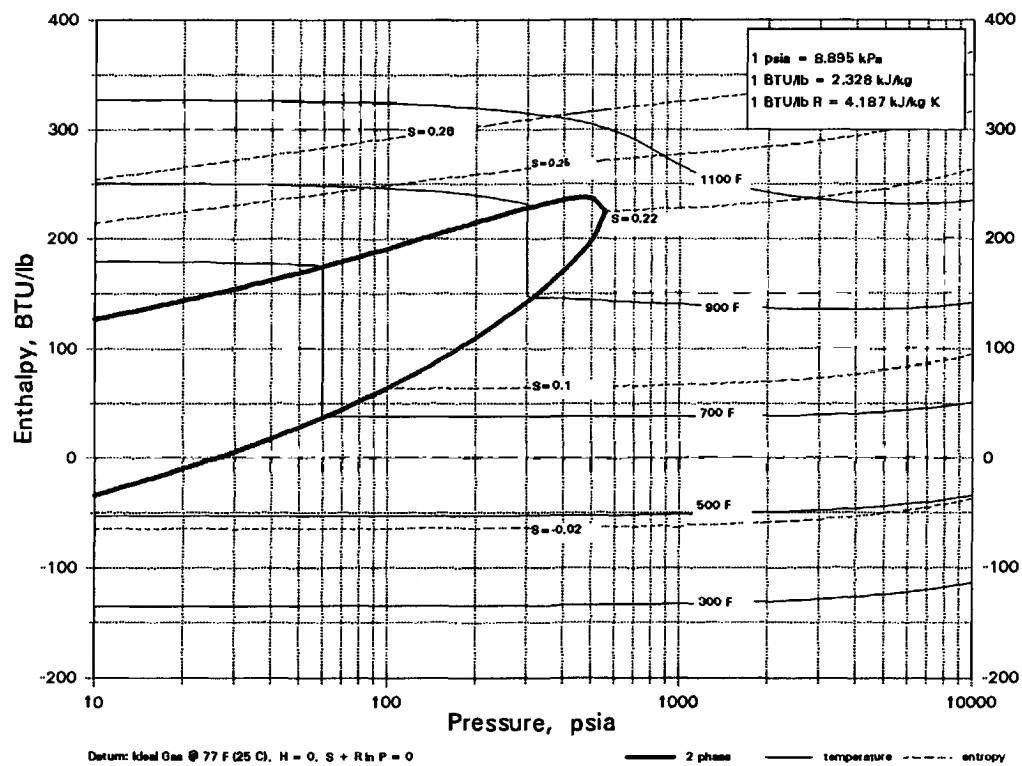
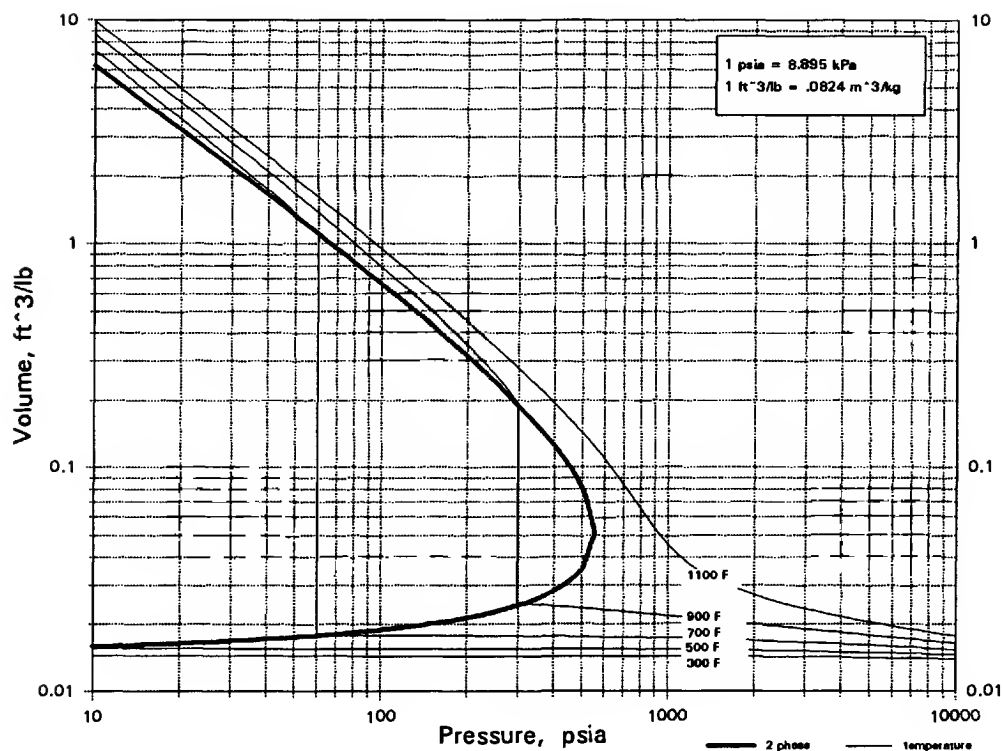
C6H4Cl2

p-DICHLOROBENZENE



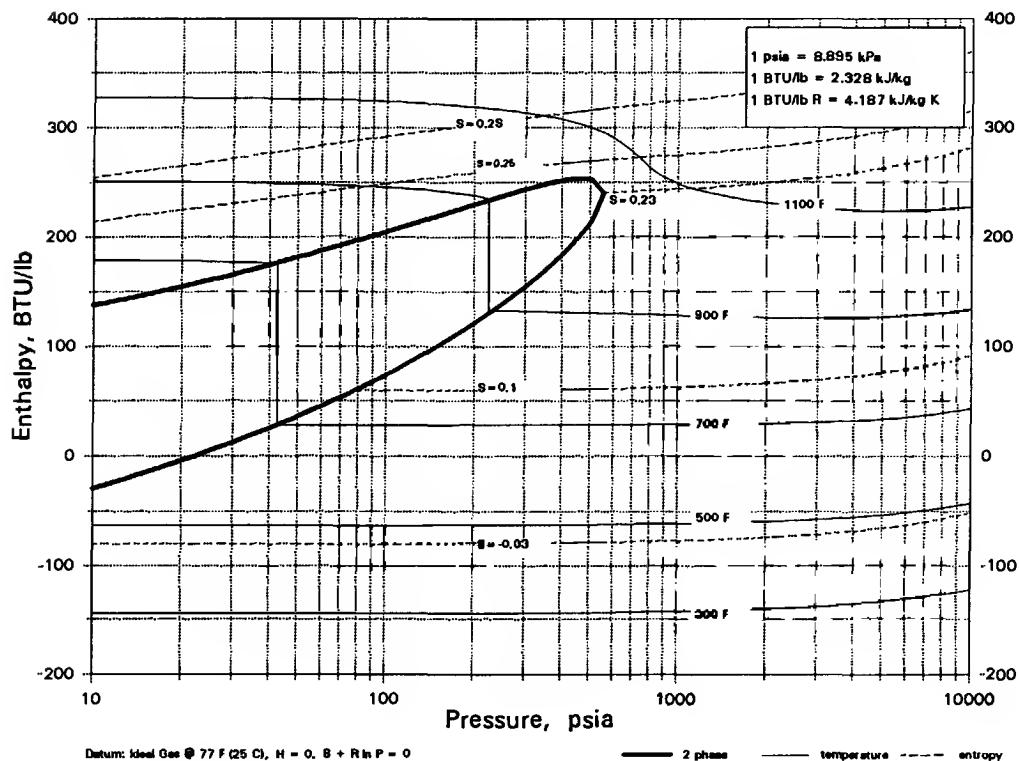
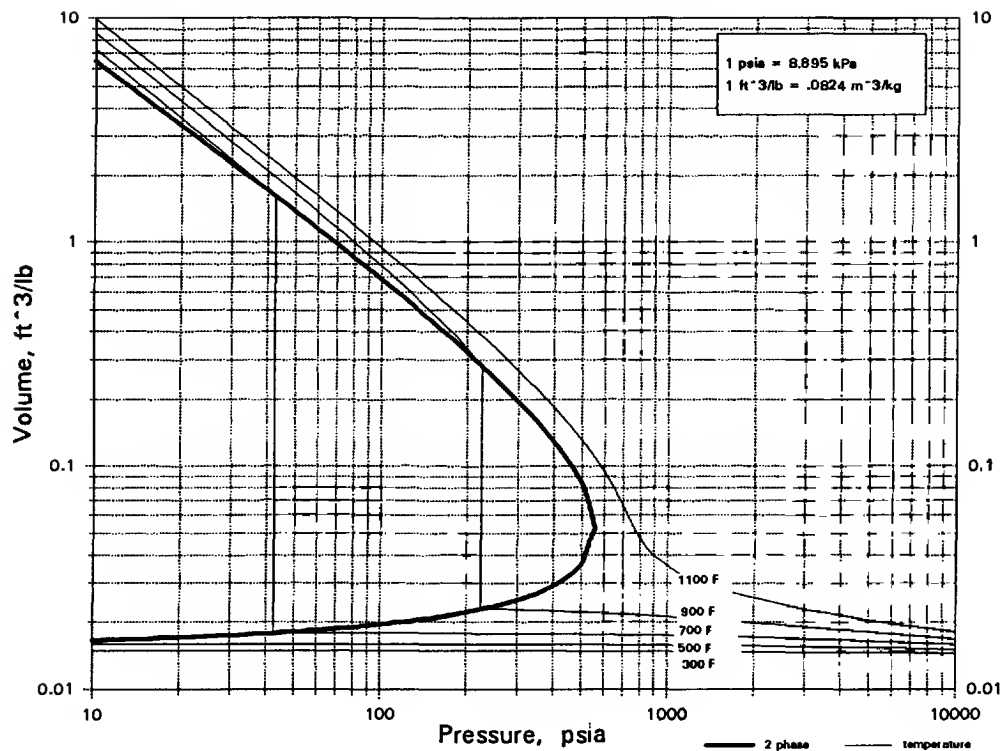
C₆H₄N₂O₄

m-DINITROBENZENE



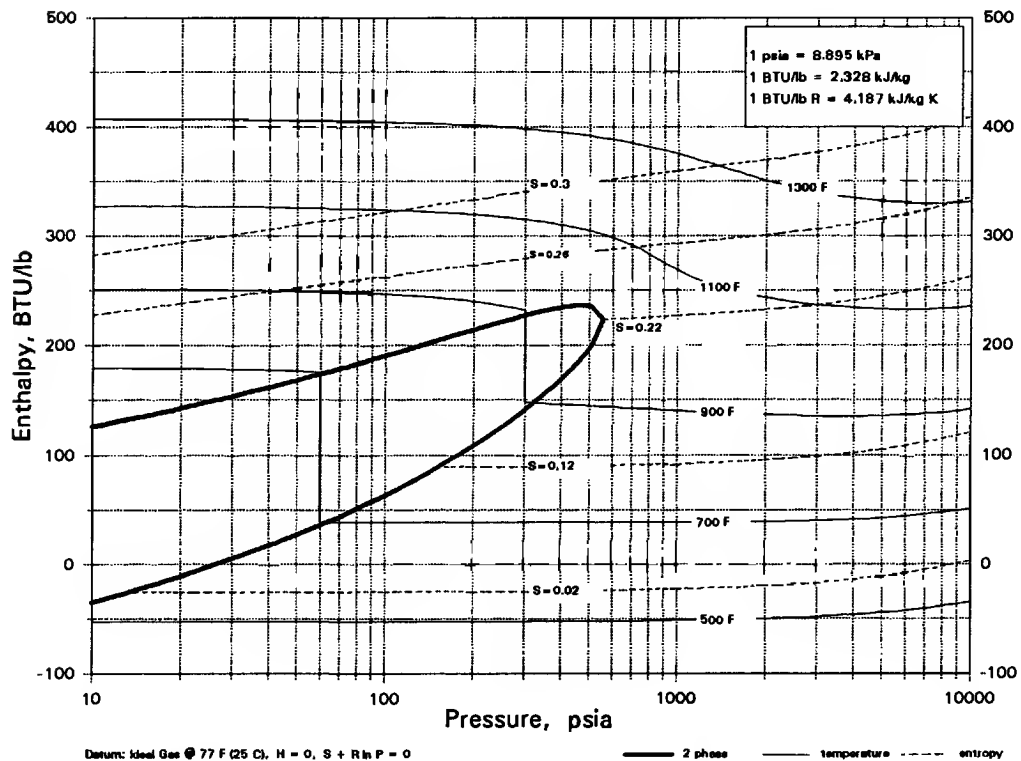
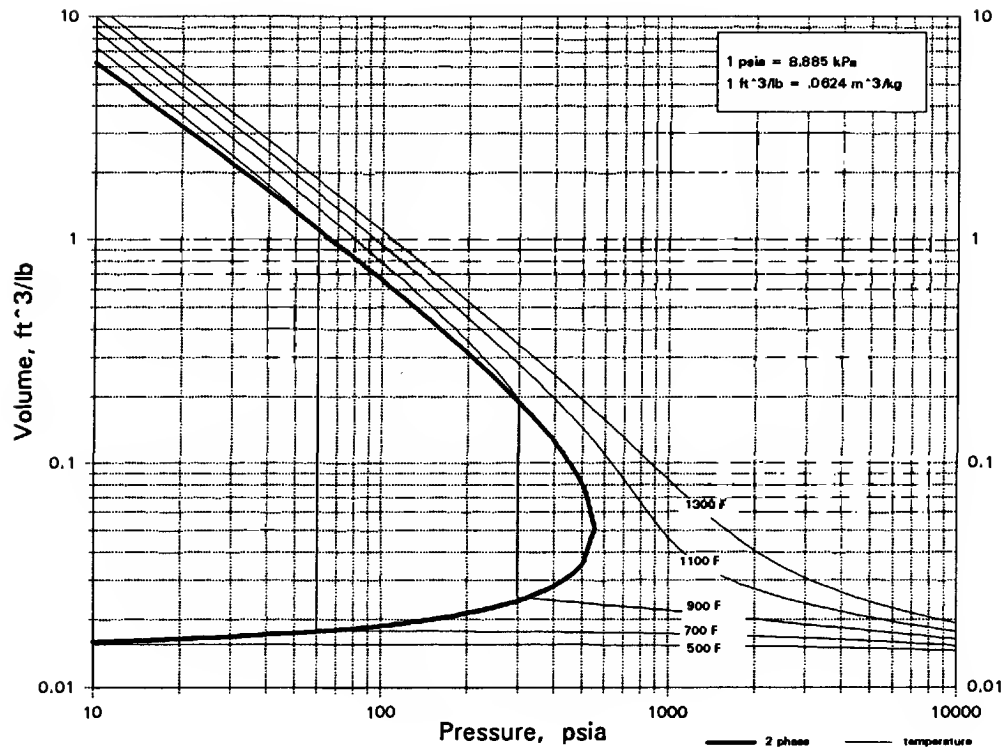
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o-DINITROBENZENE



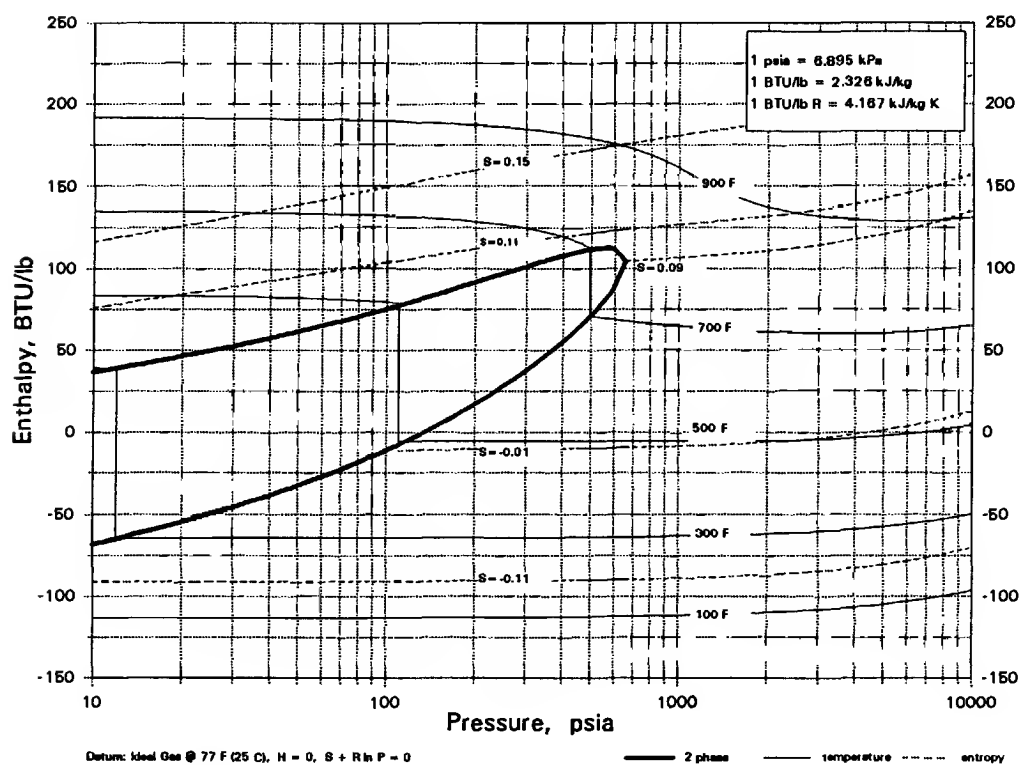
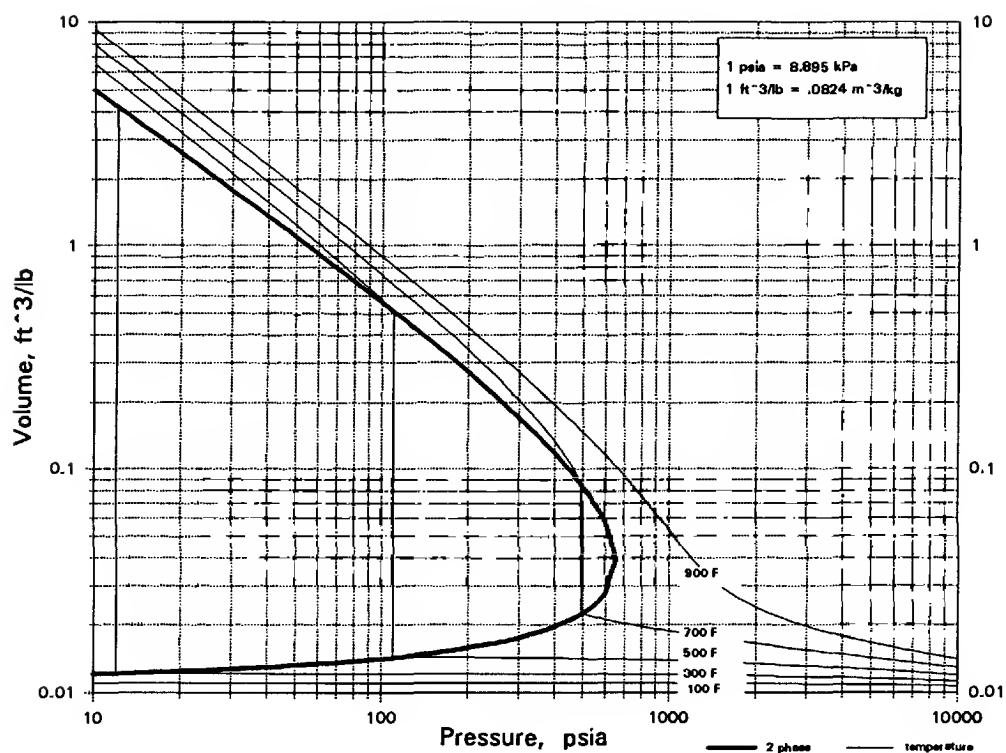
C₆H₄N₂O₄

p-DINITROBENZENE



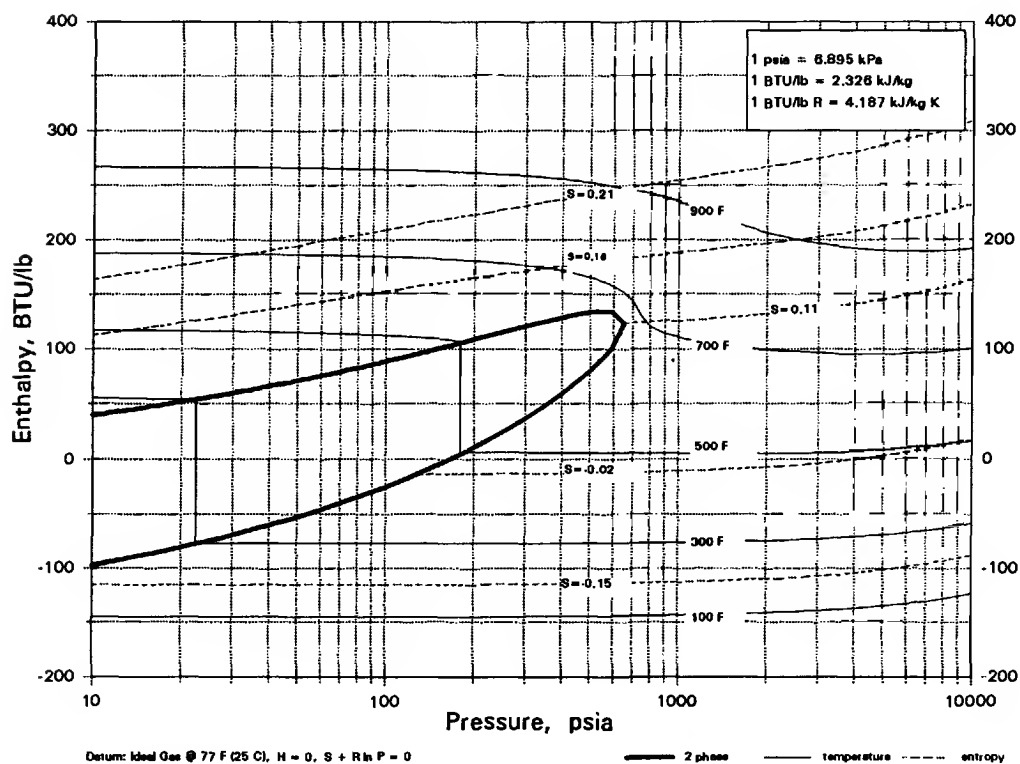
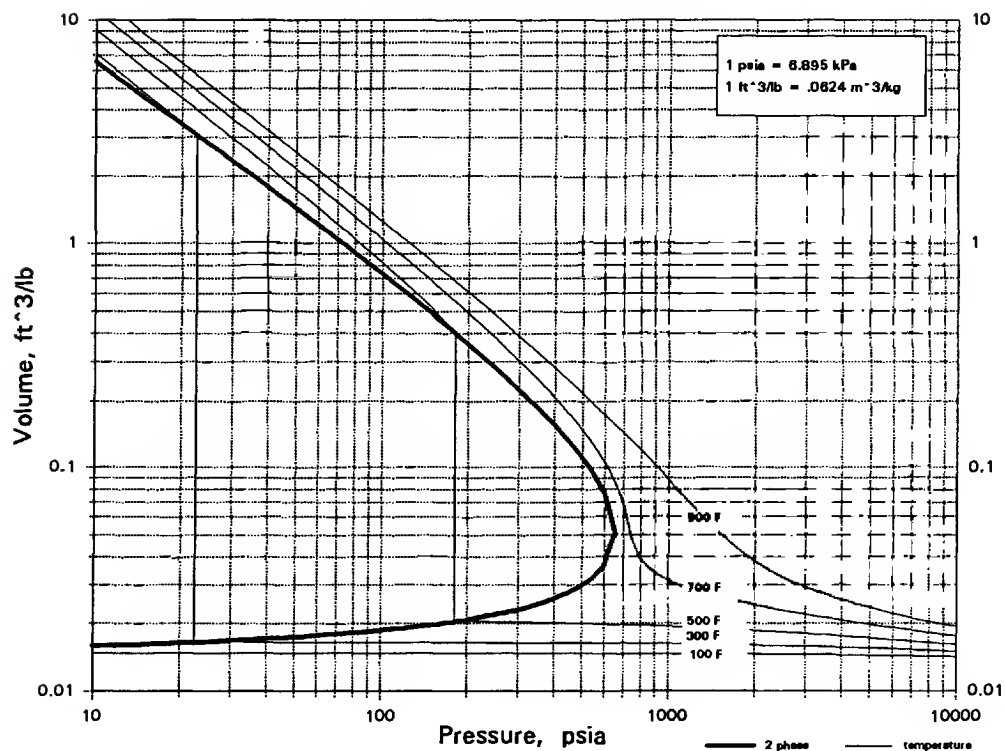
C6H5Br

BROMOBENZENE



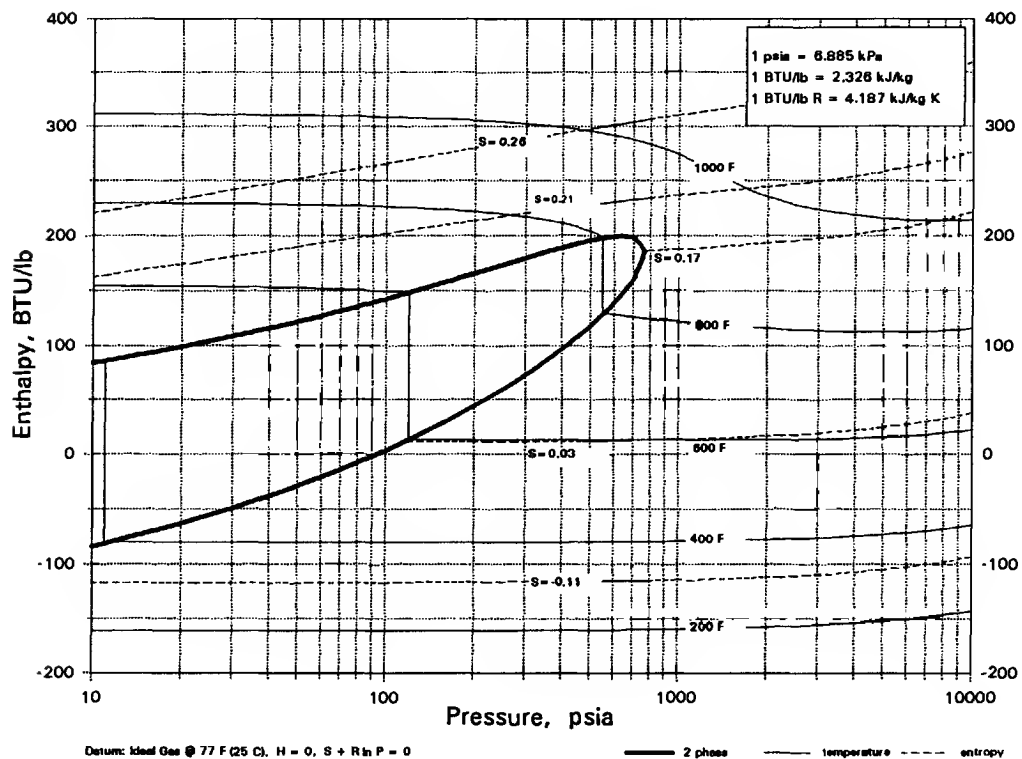
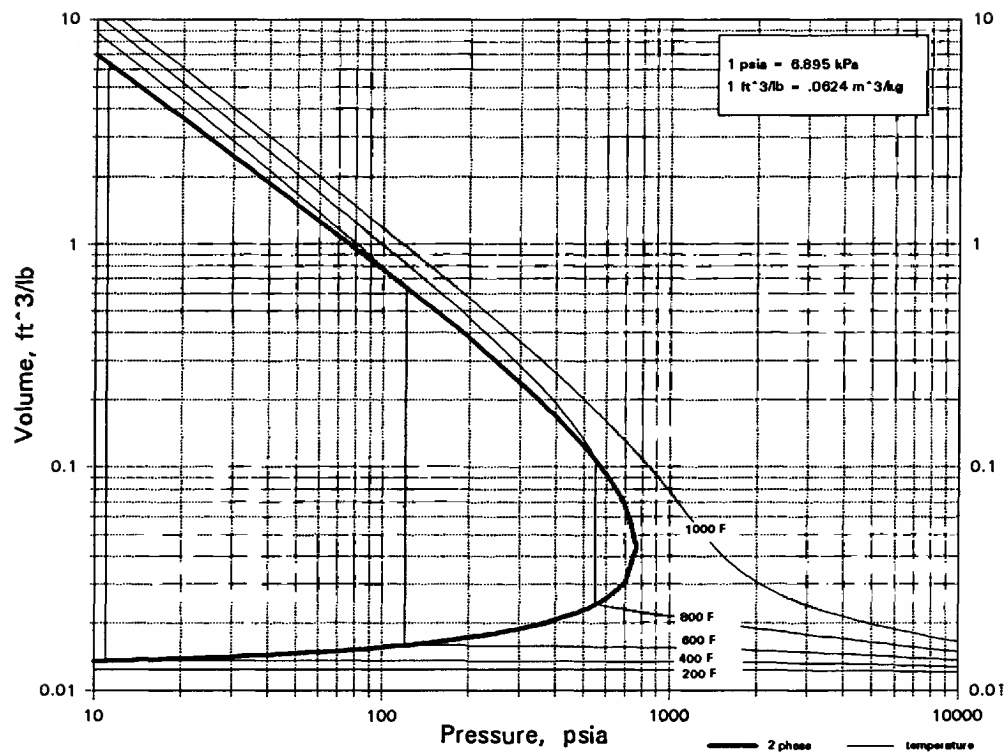
C6H5Cl

MONOCHLOROBENZENE



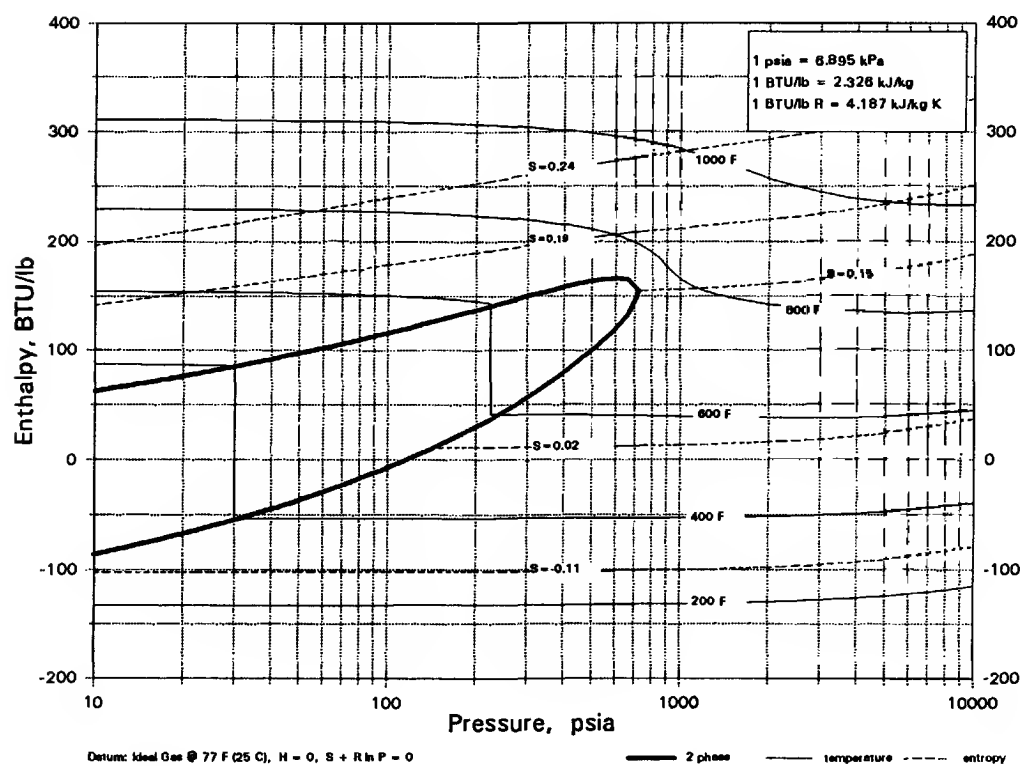
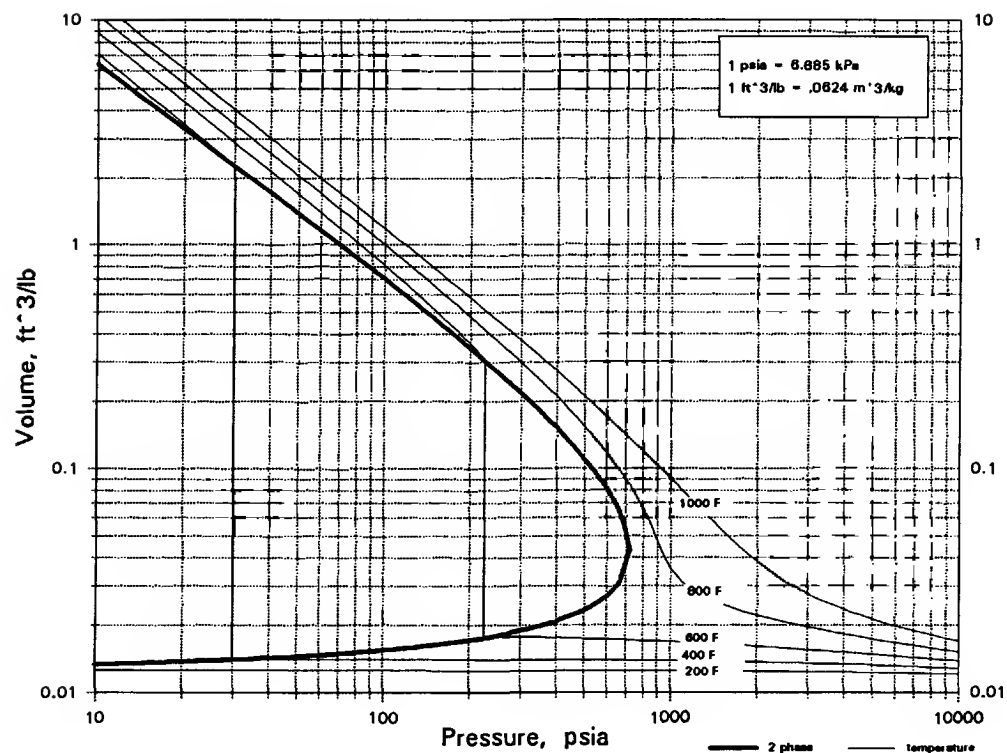
C₆H₅ClO

m-CHLOROPHENOL



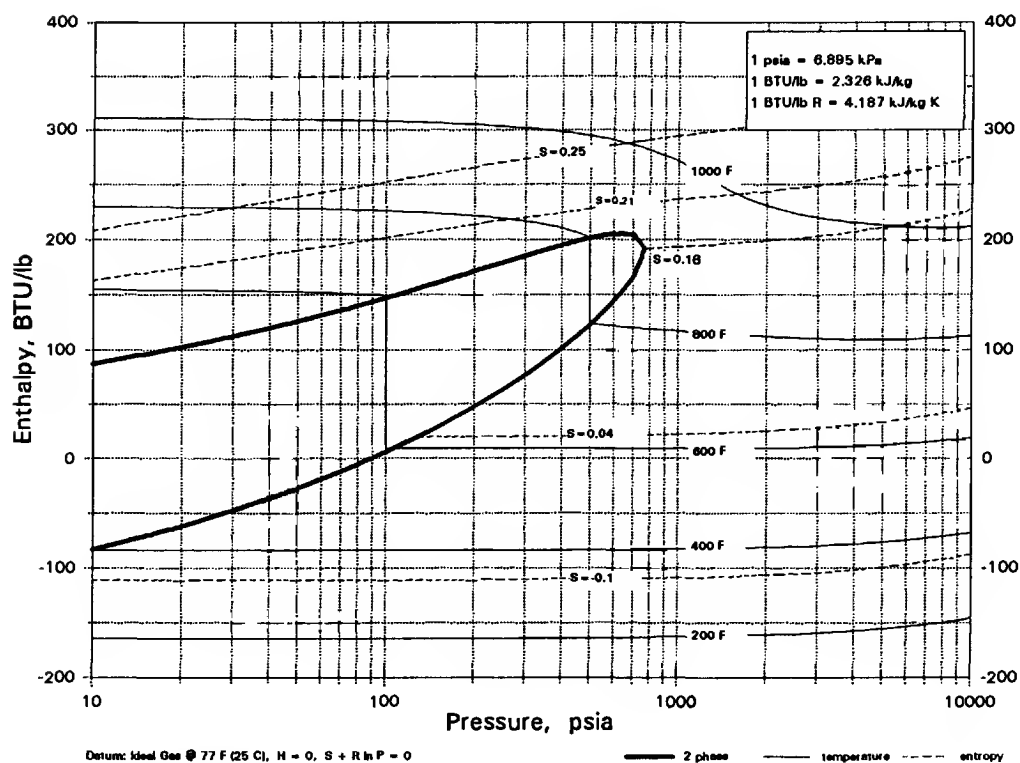
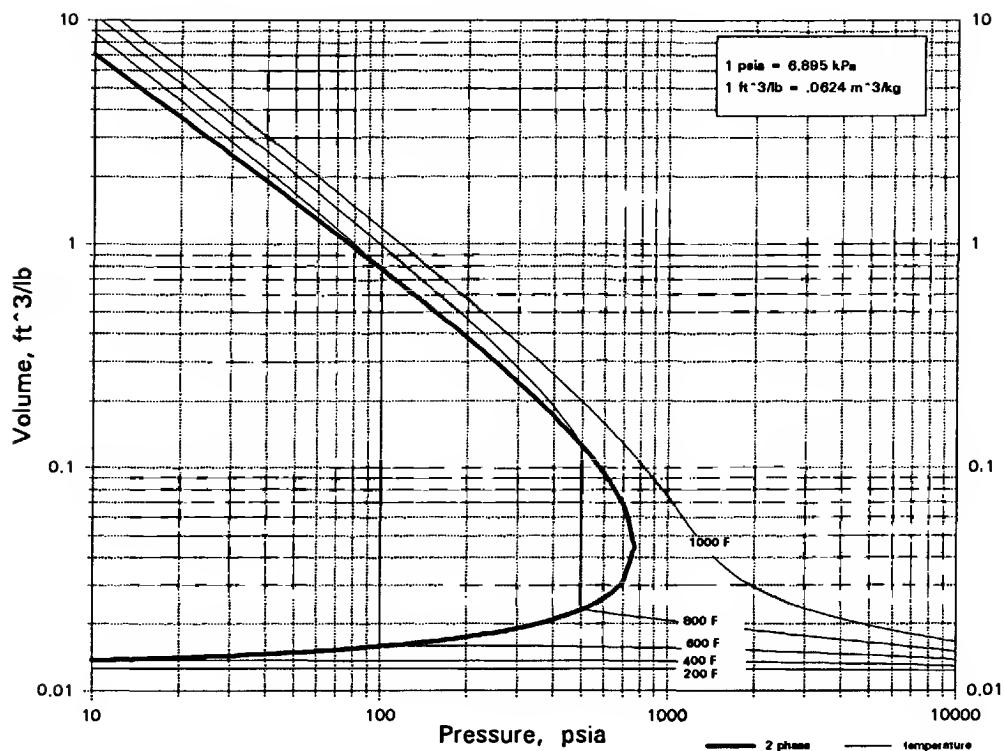
C6H5ClO

o-CHLOROPHENOL



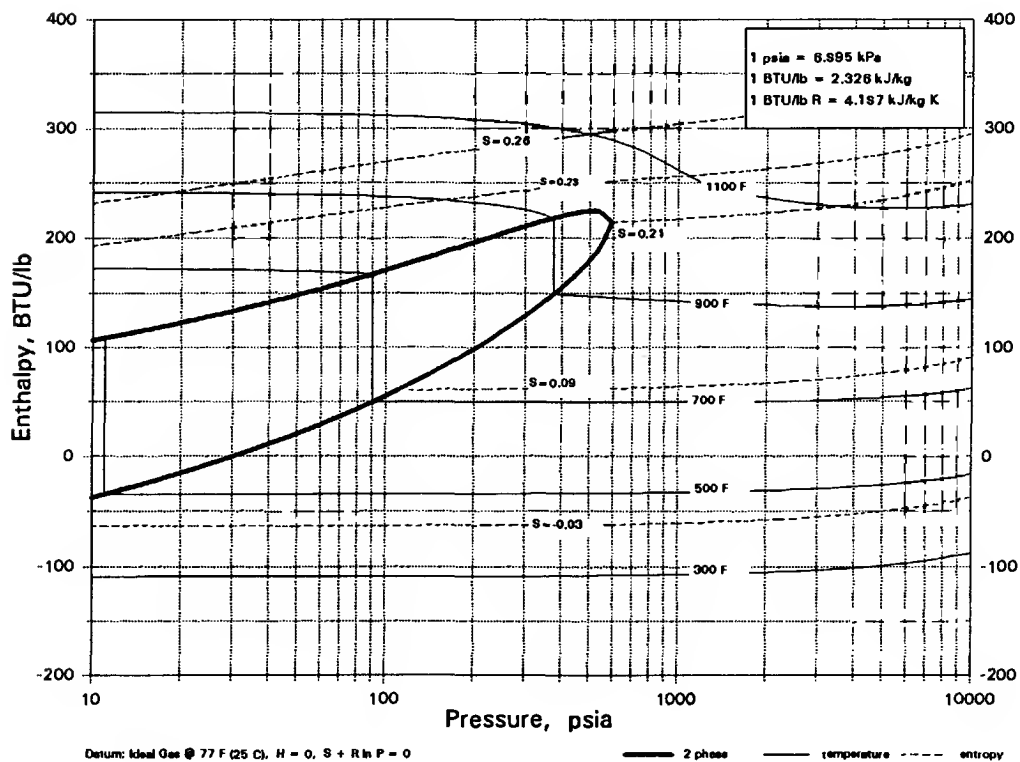
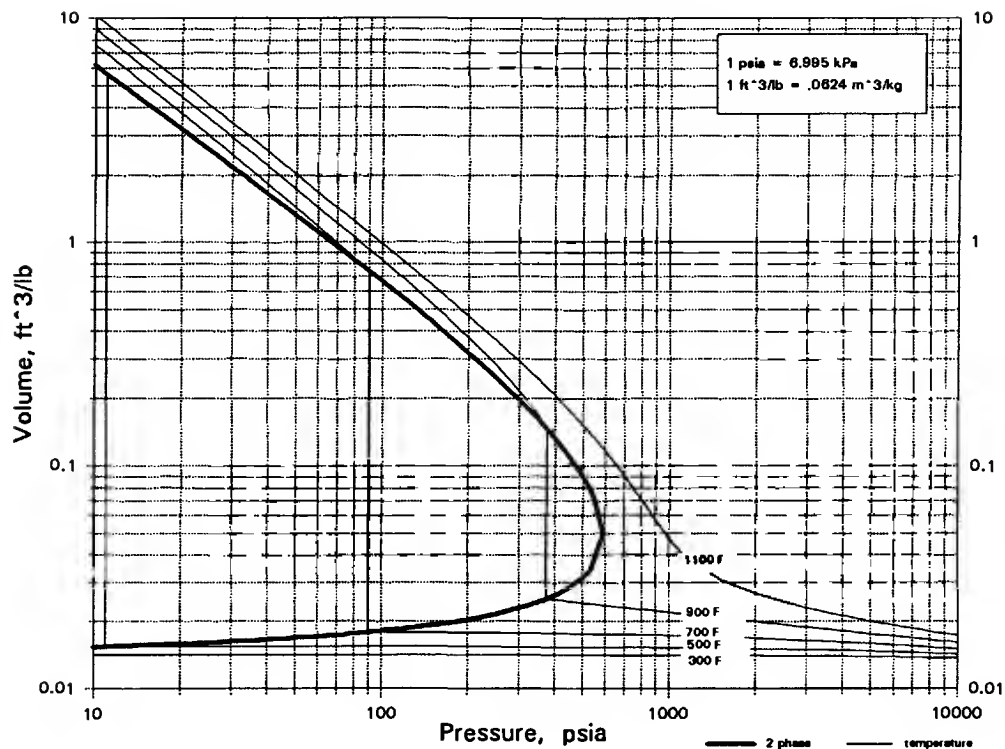
C6H5ClO

p-CHLOROPHENOL



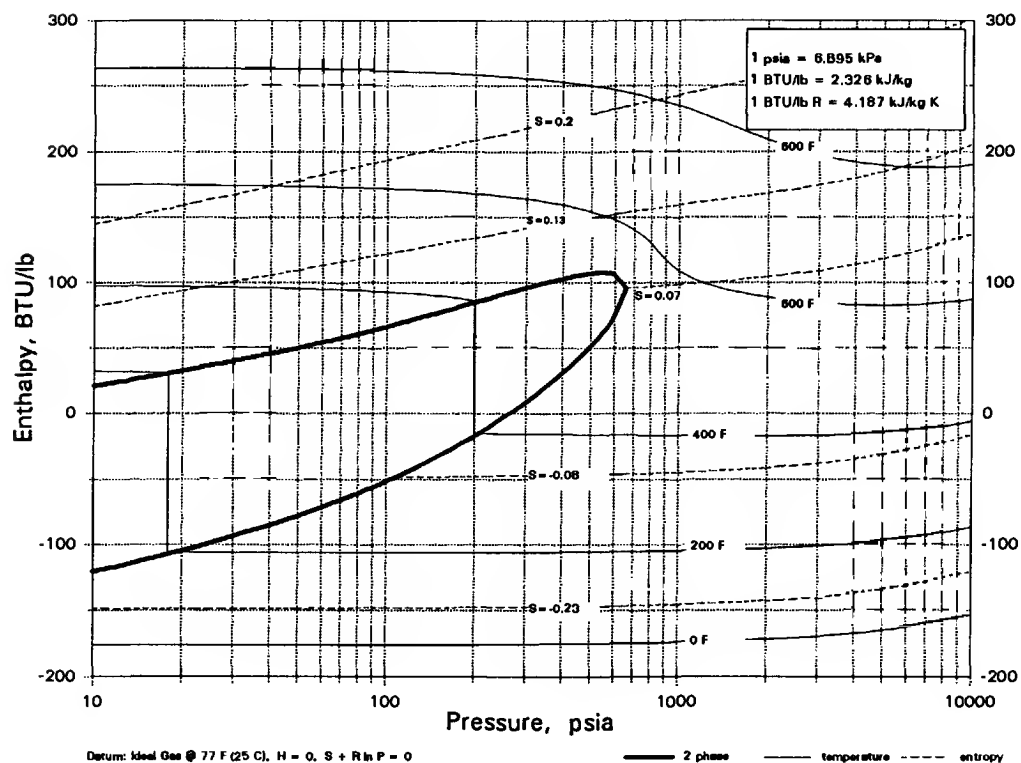
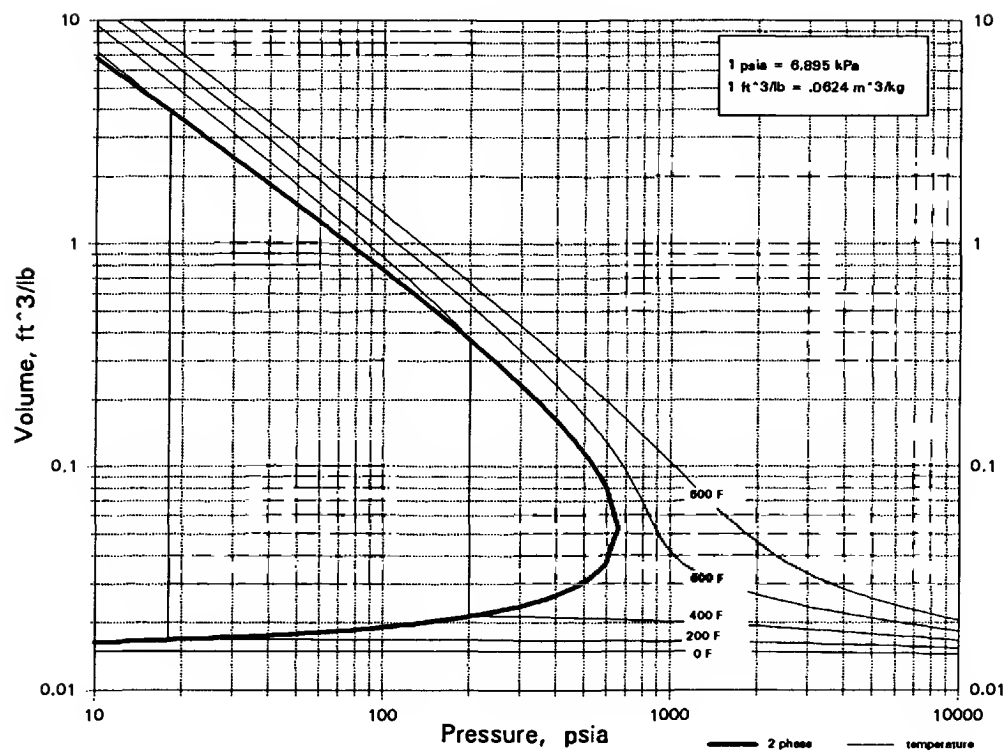
C6H5Cl2N

3-4-DICHLOROANILINE



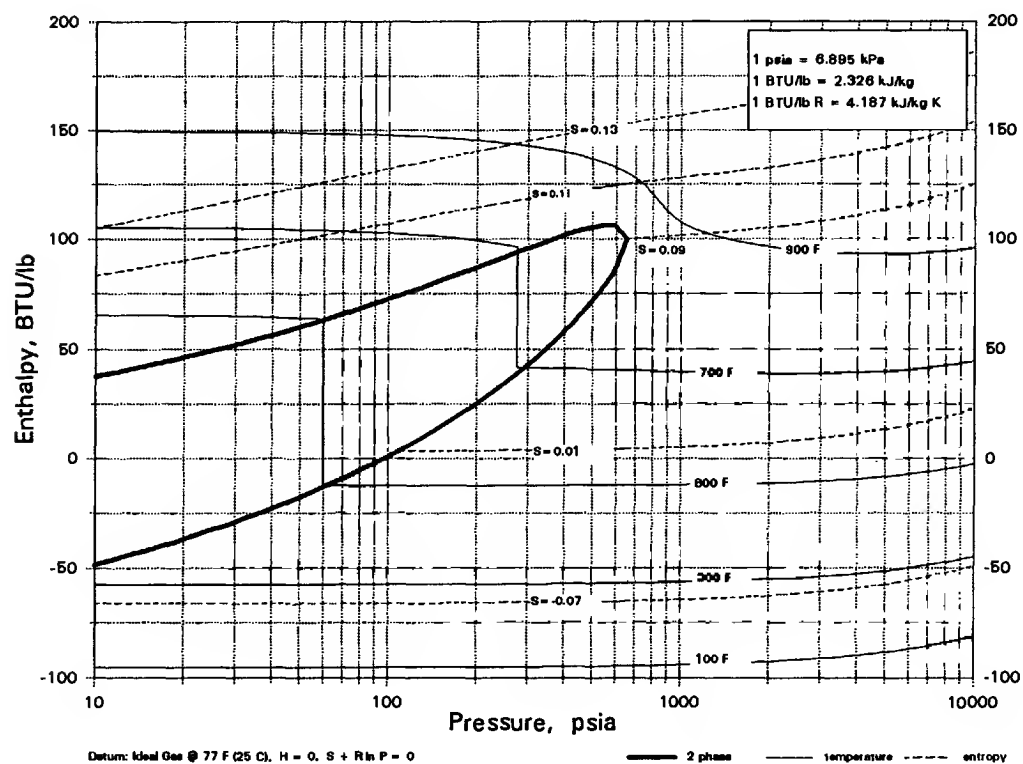
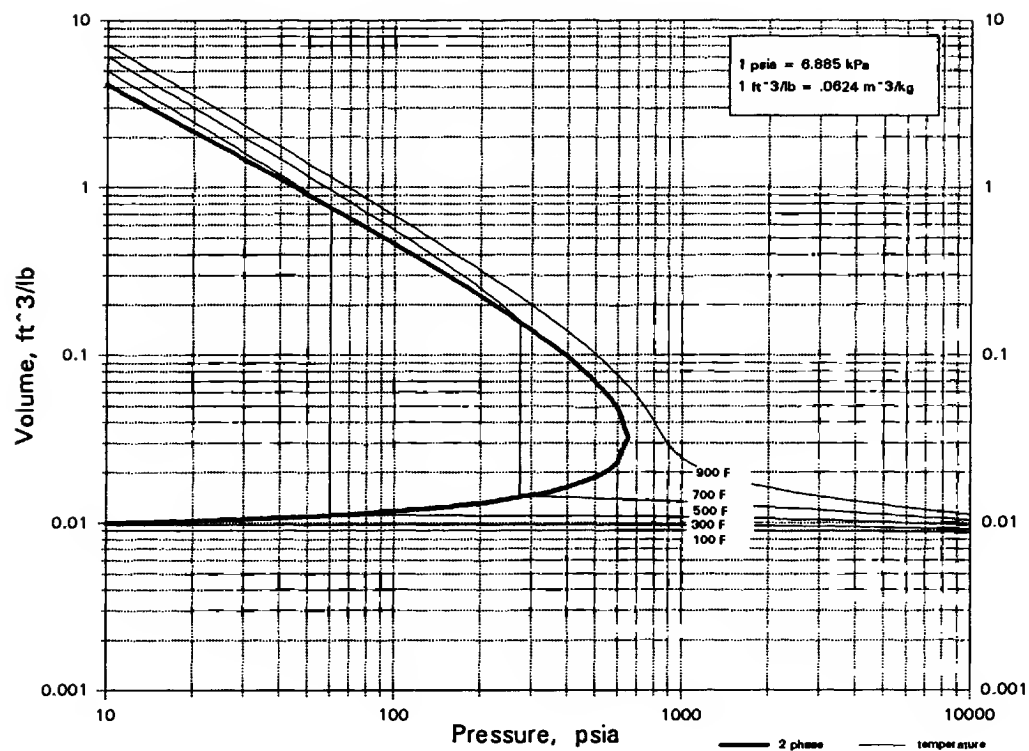
C6H5F

FLUOROBENZENE

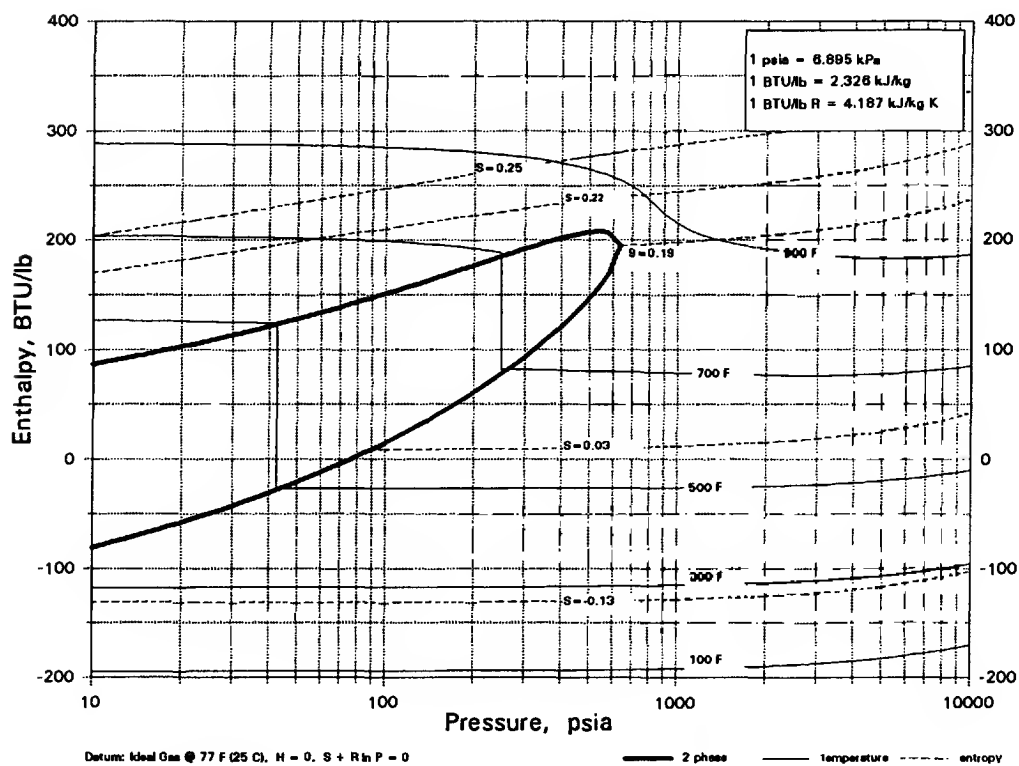
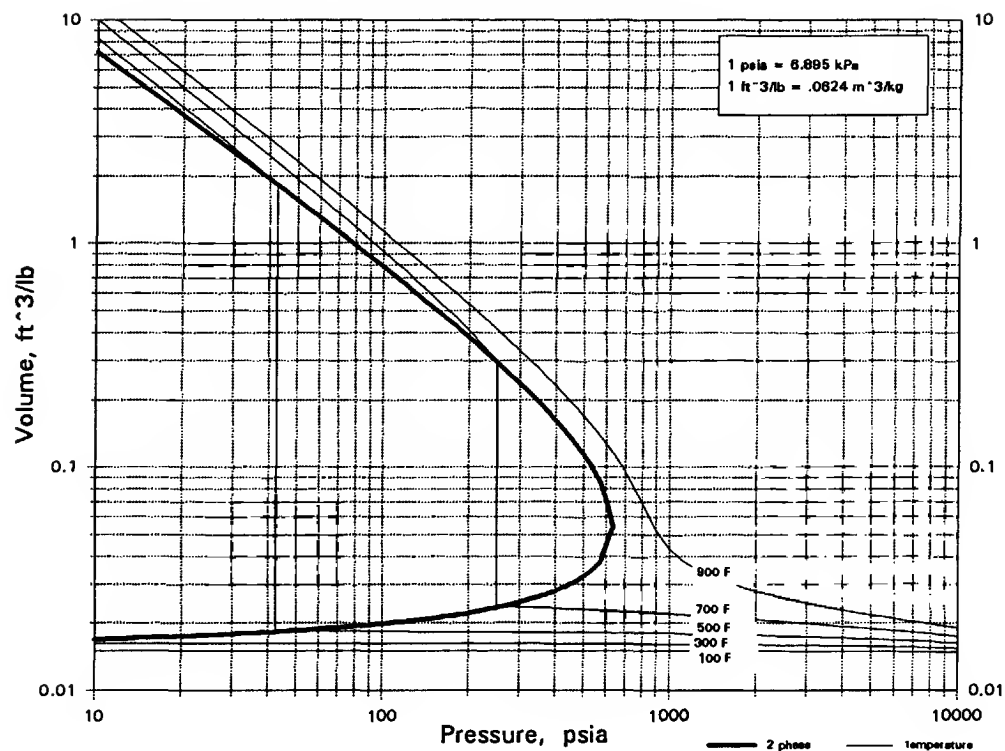


C6H5I

IODOBENZENE

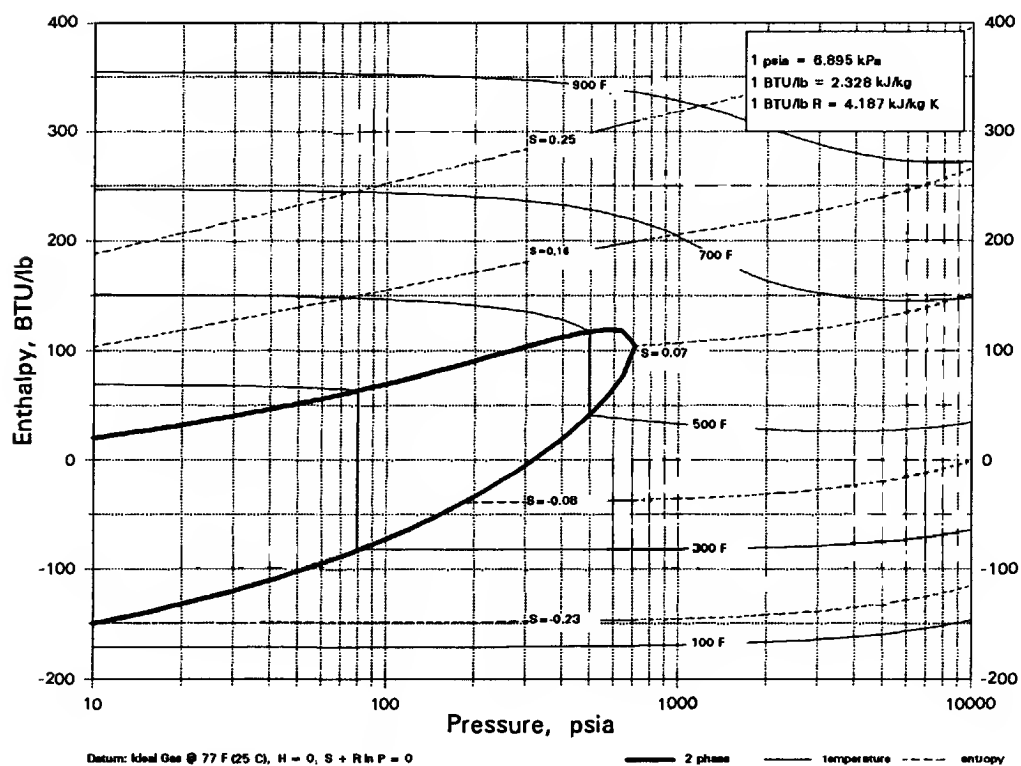
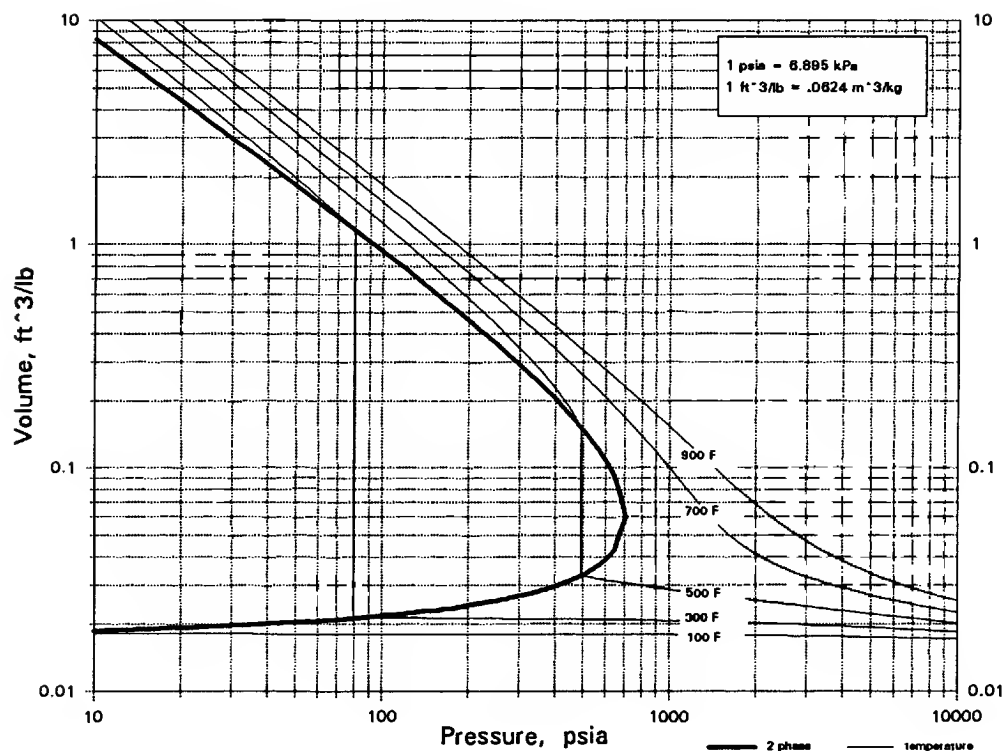


C6H5NO2 NITROBENZENE



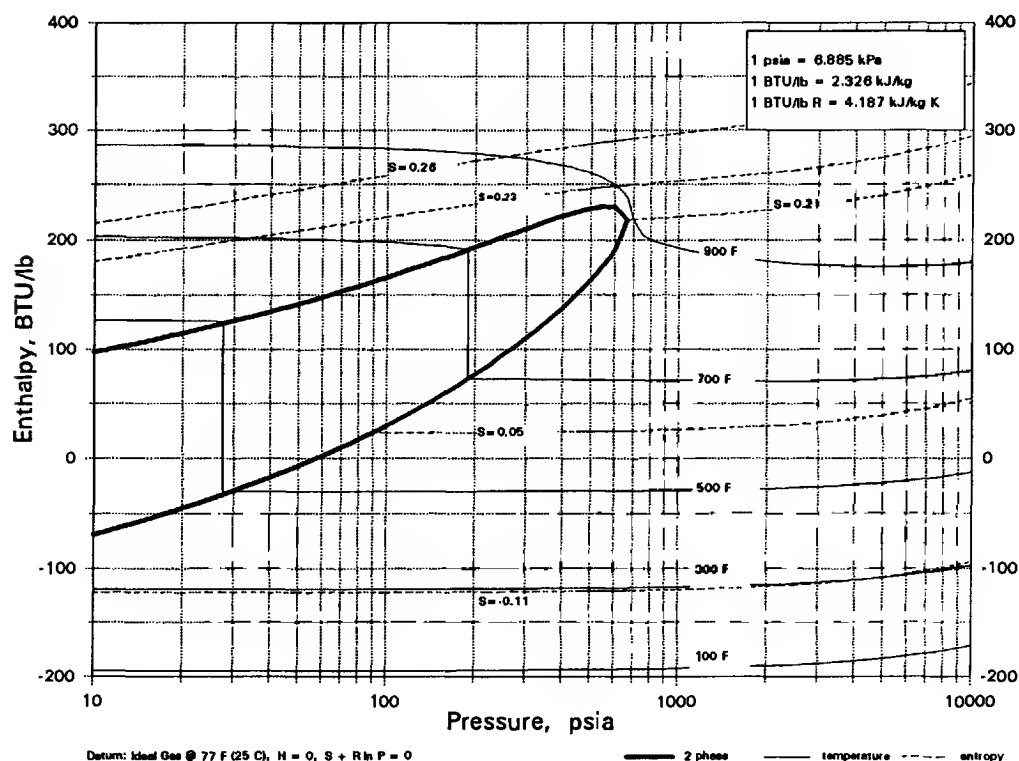
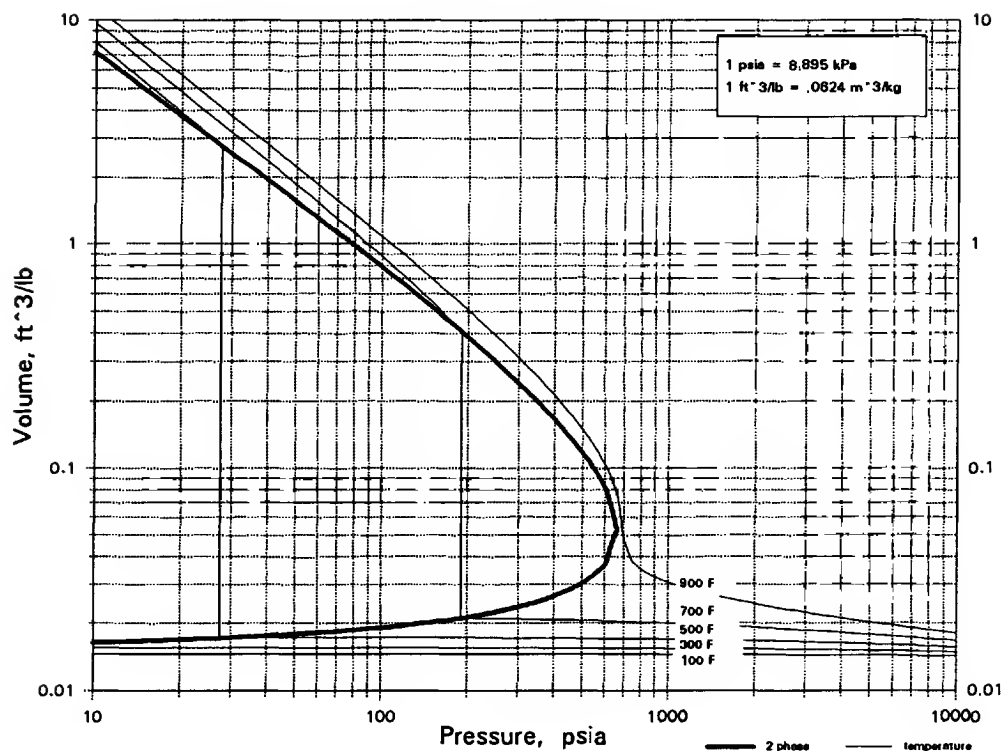
C6H6

BENZENE



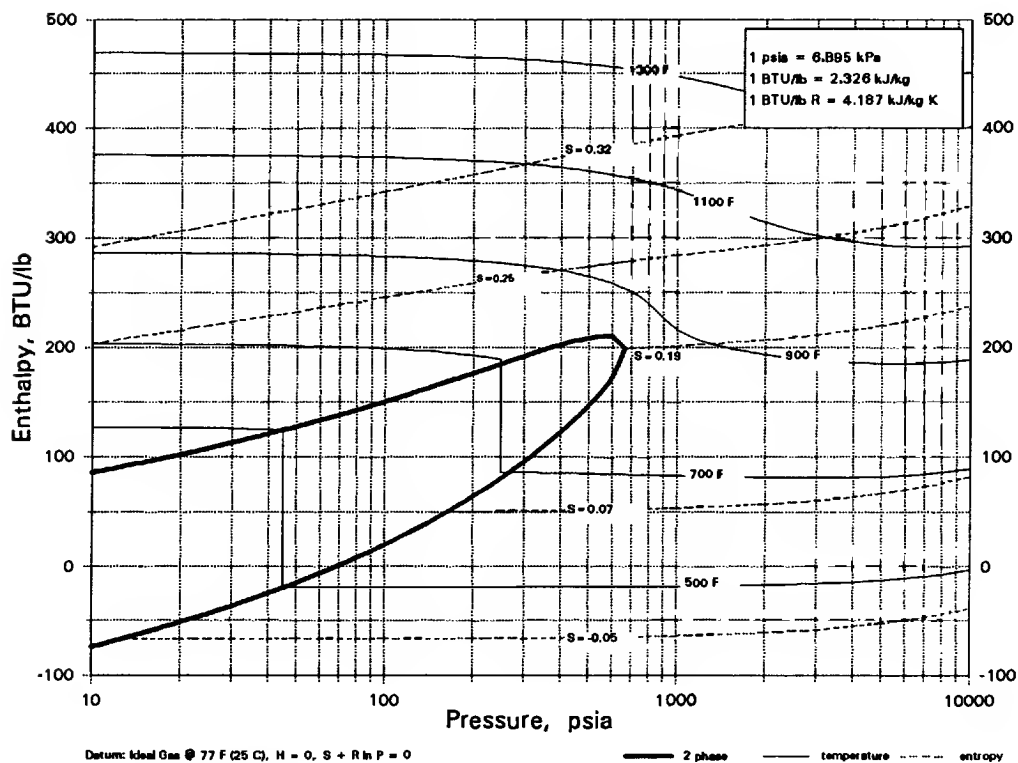
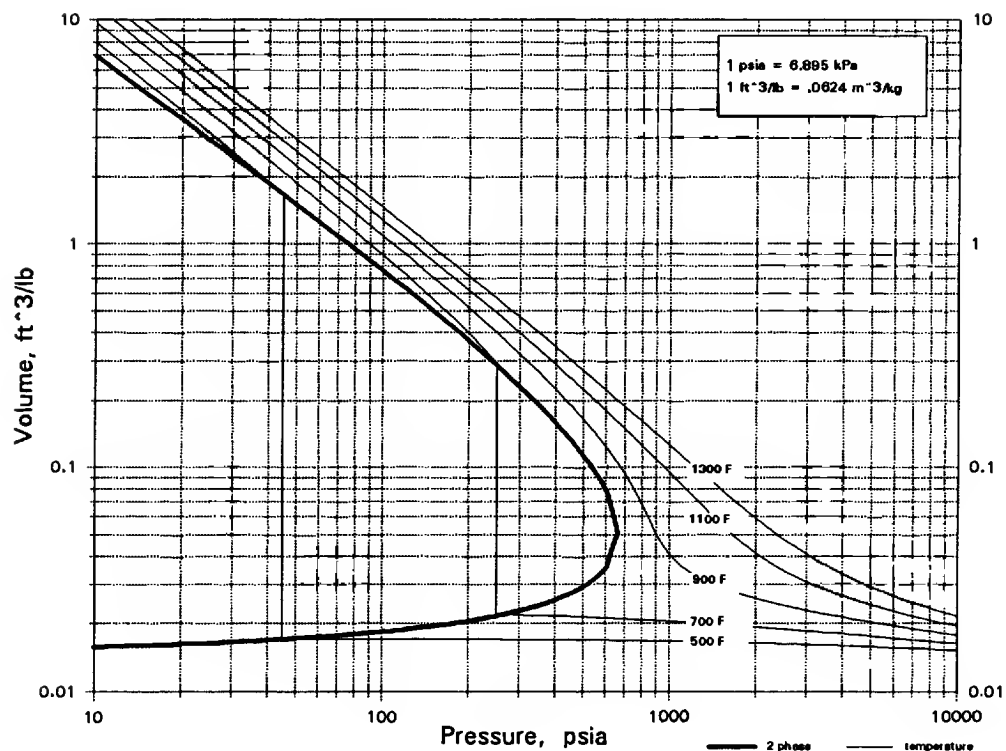
C6H6ClN

m-CHLOROANILINE



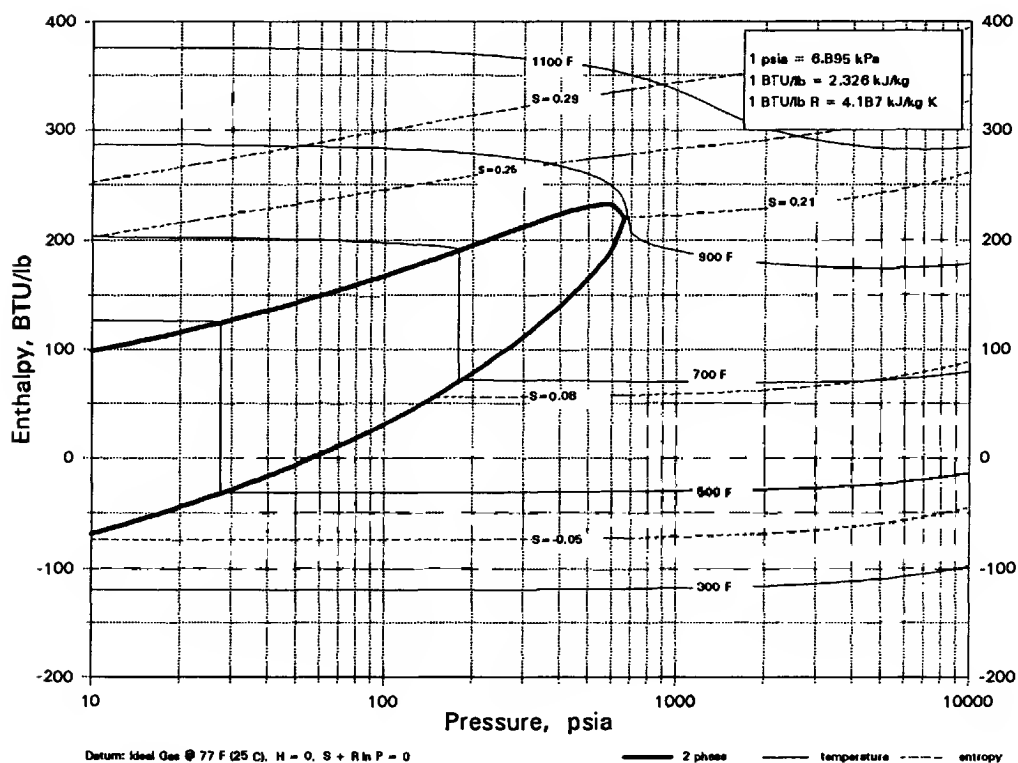
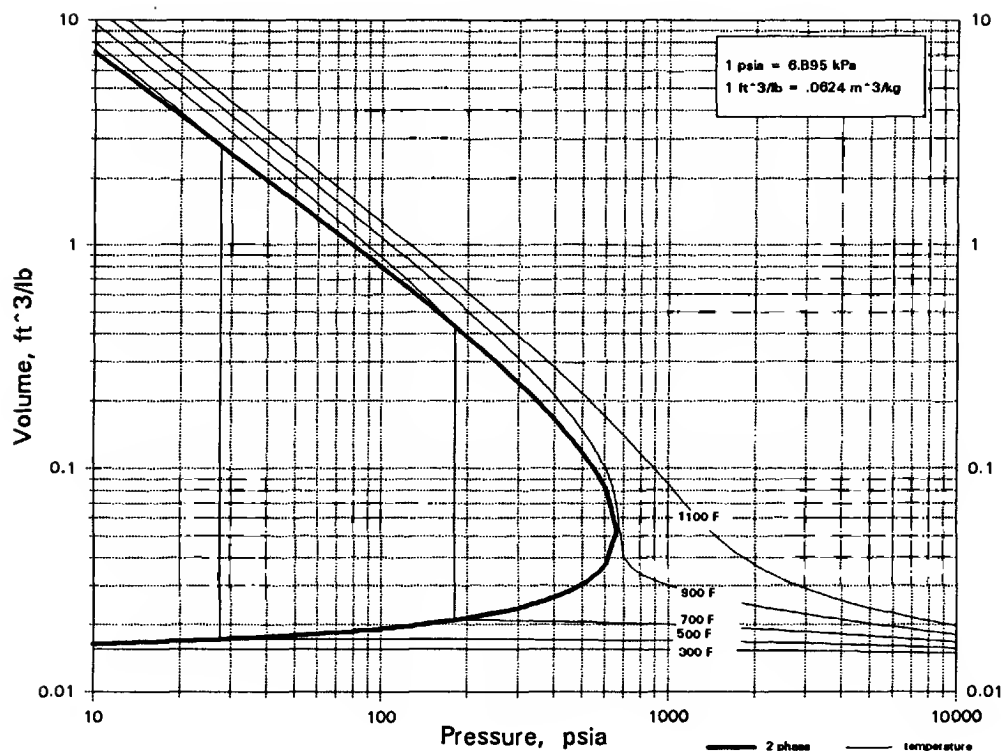
C6H6ClN

o-CHLOROANILINE



C6H6ClN

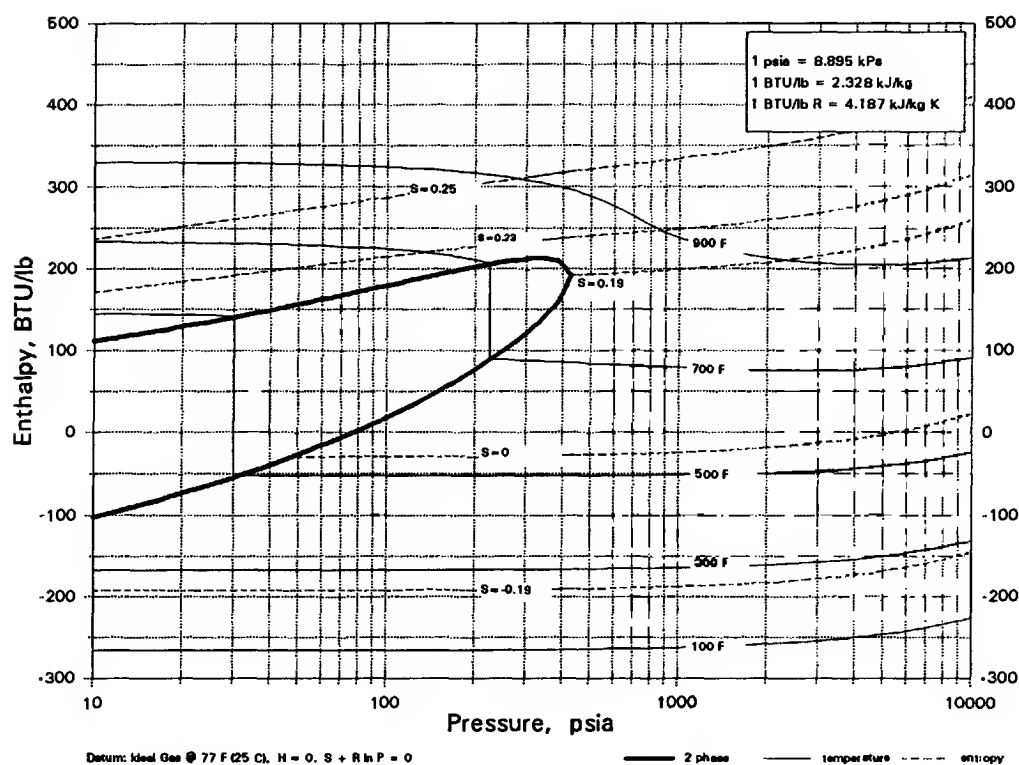
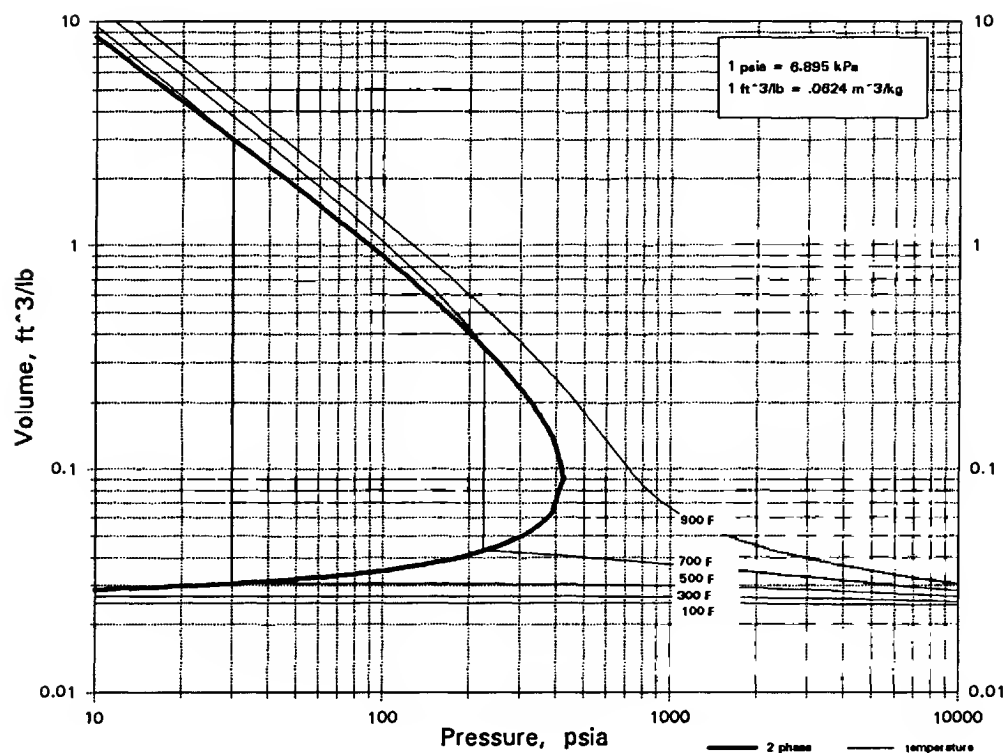
p-CHLOROANILINE



Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

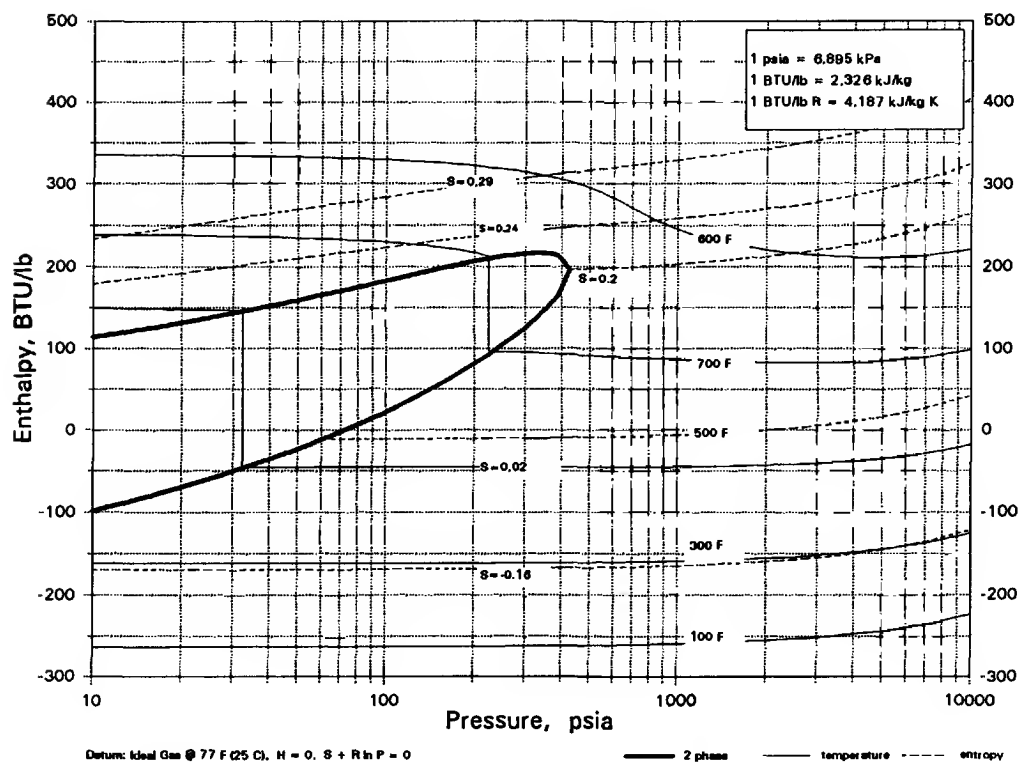
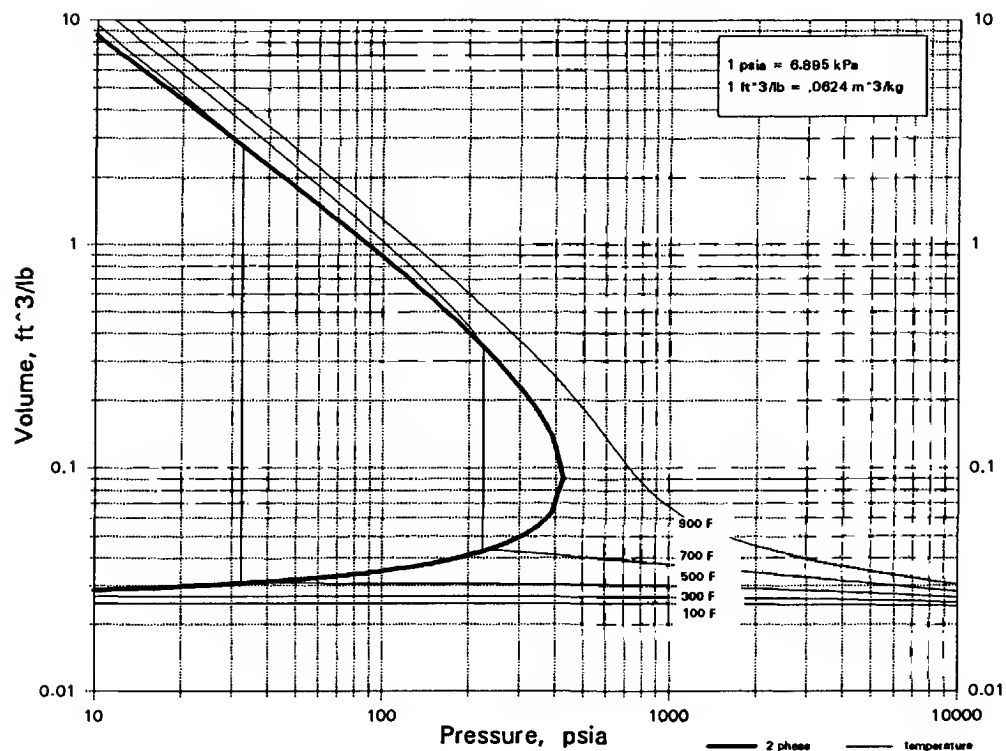
C6H6N2

cis-DICYANO-1-BUTENE



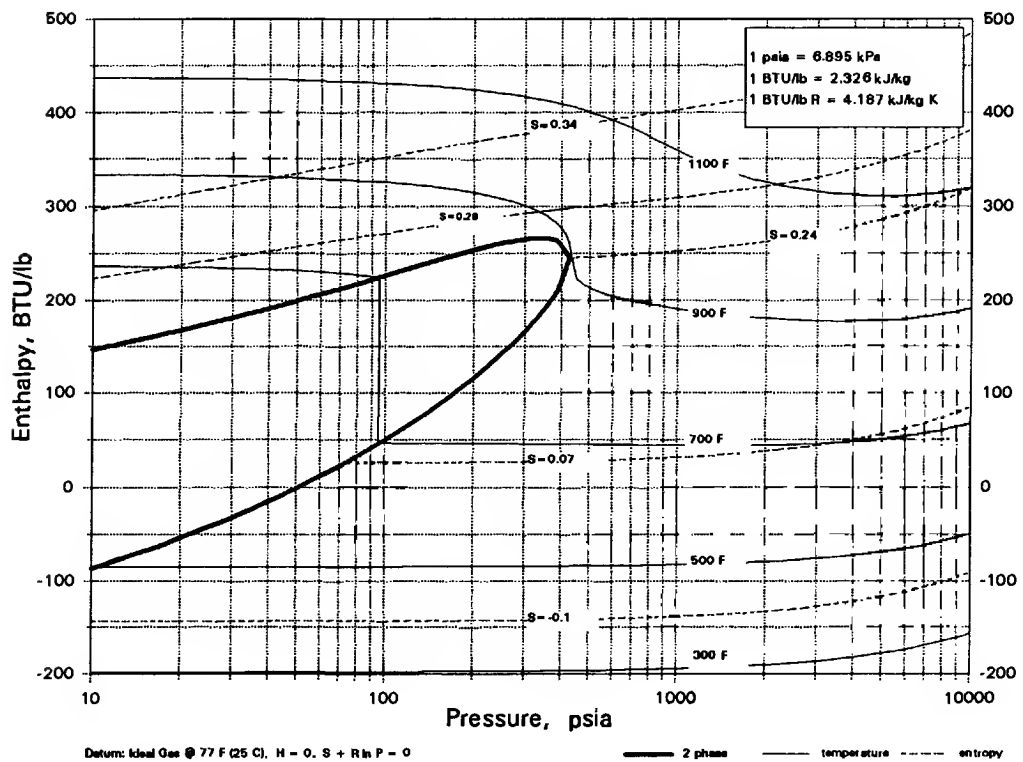
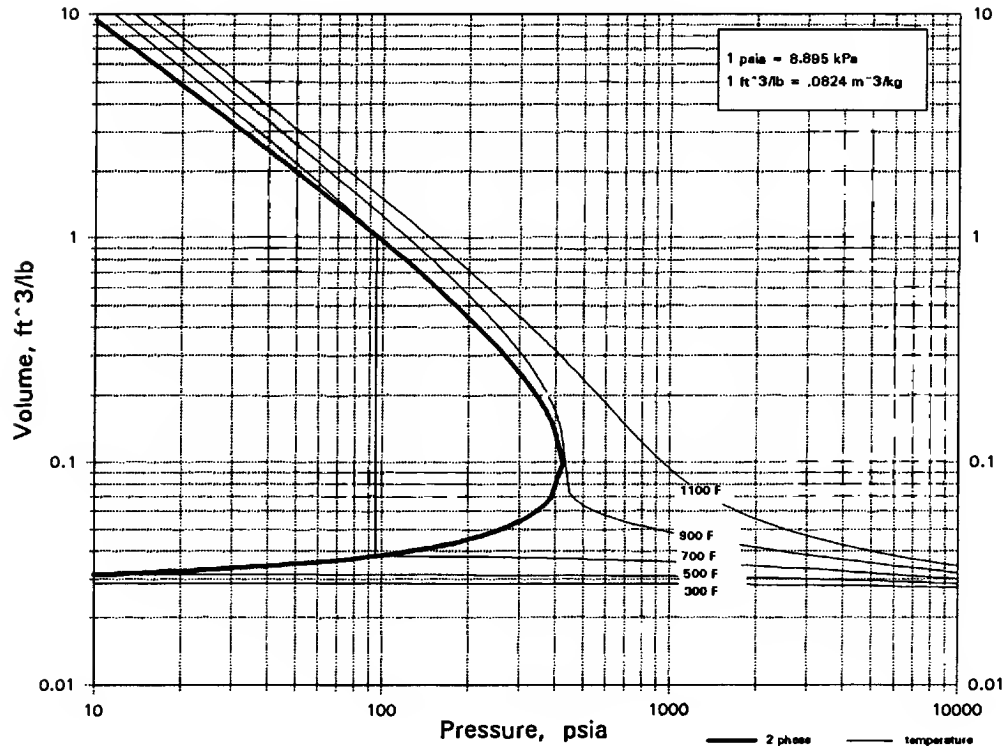
C6H6N2

trans-DICYANO-1-BUTENE

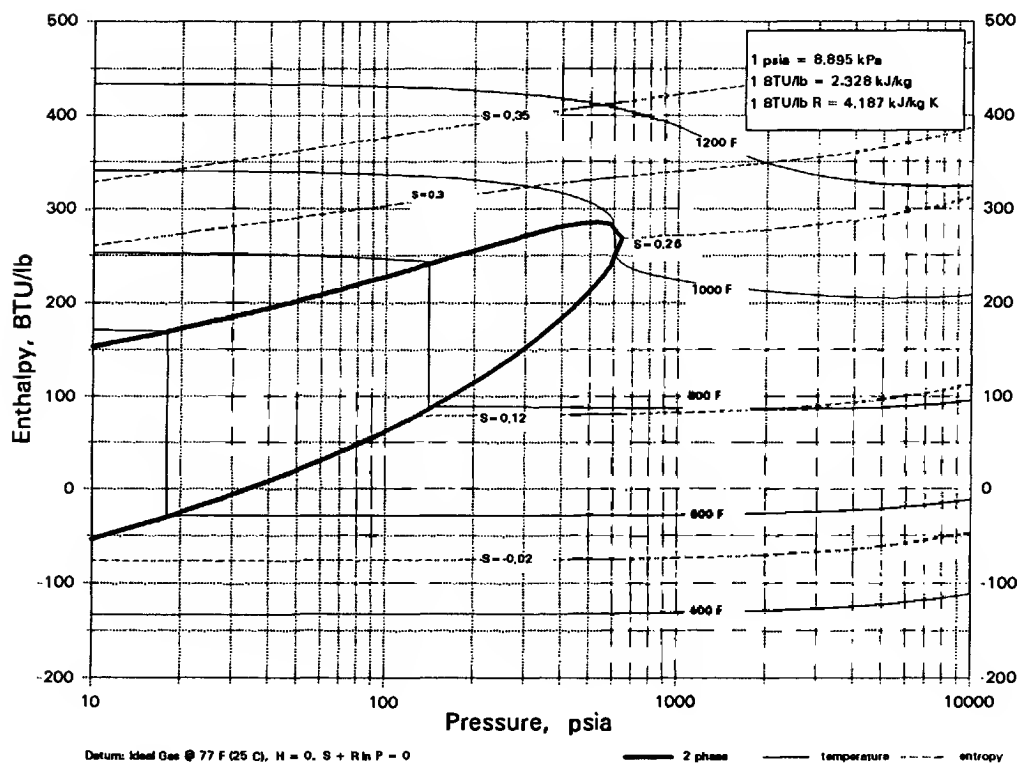
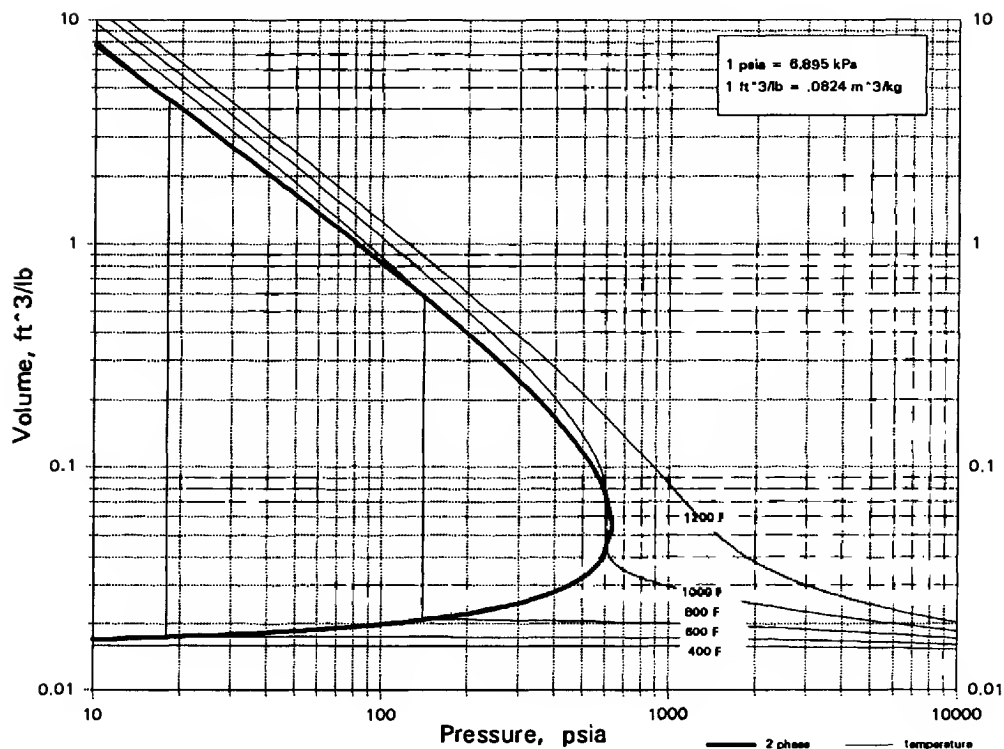


C6H6N2

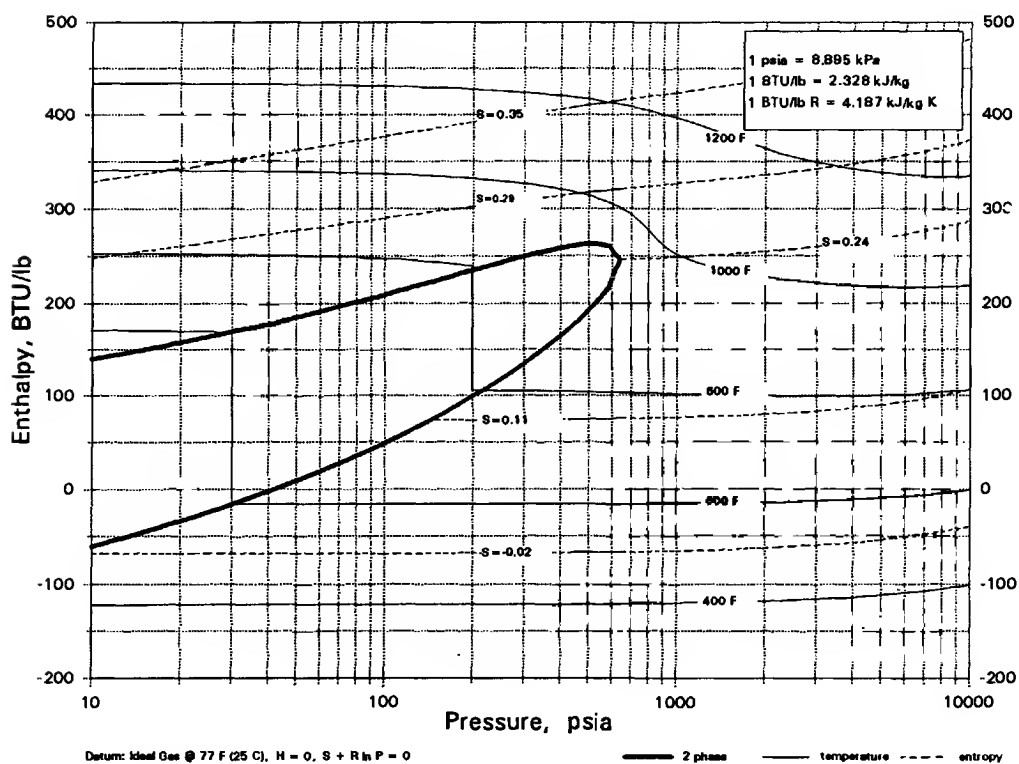
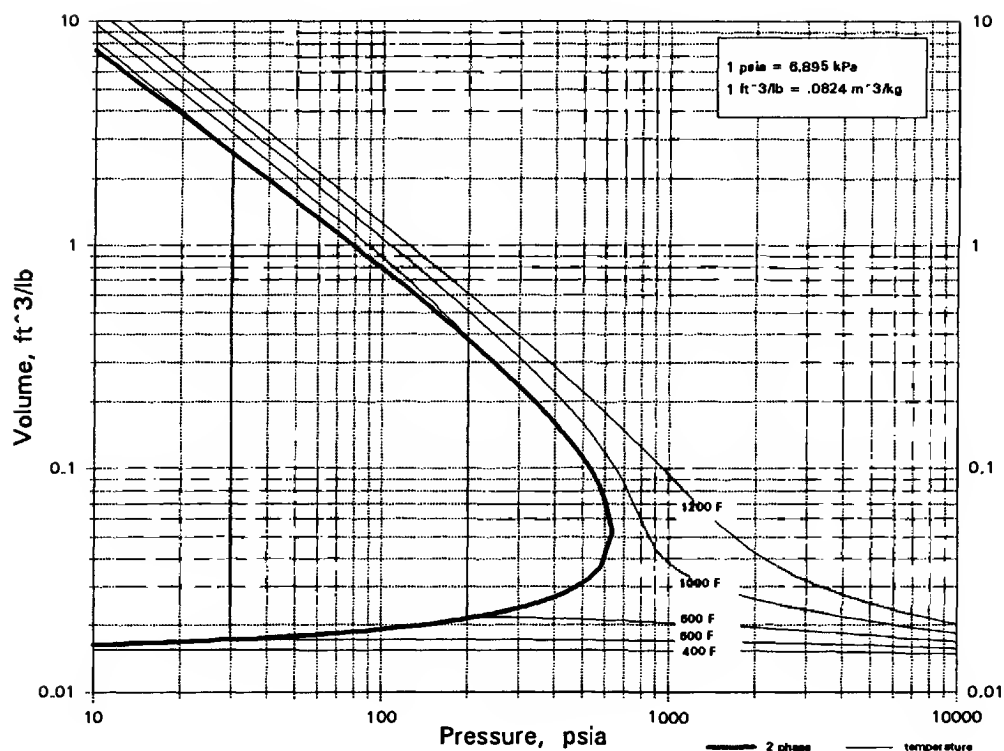
1-4-DICYANO-2-BUTENE



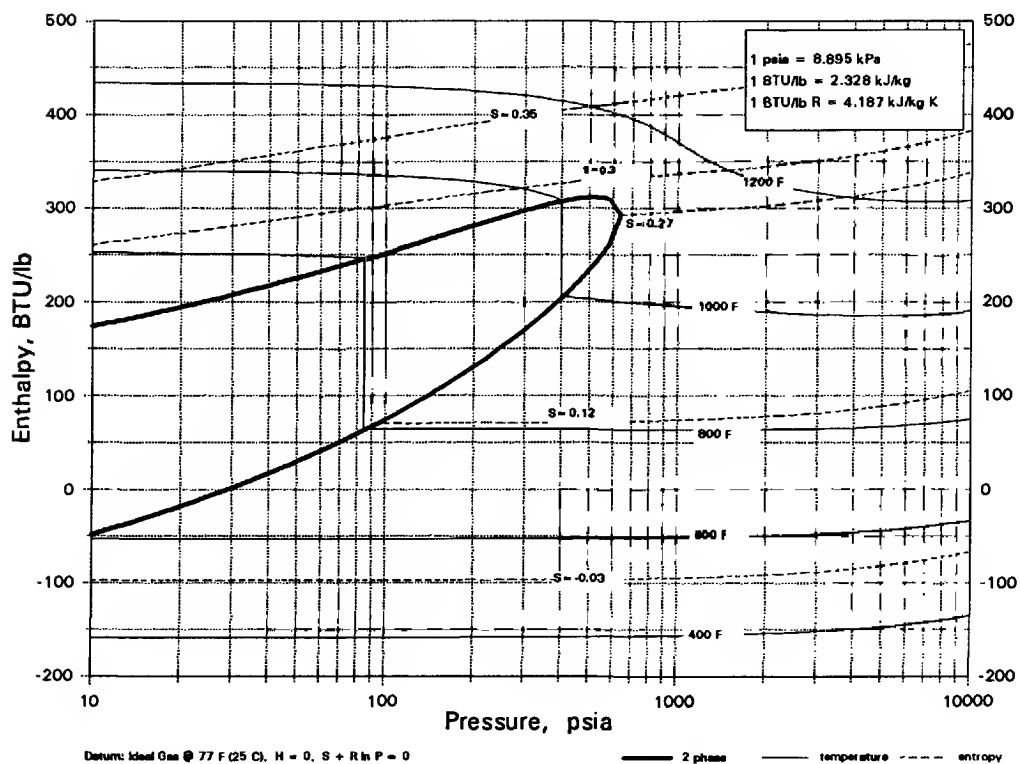
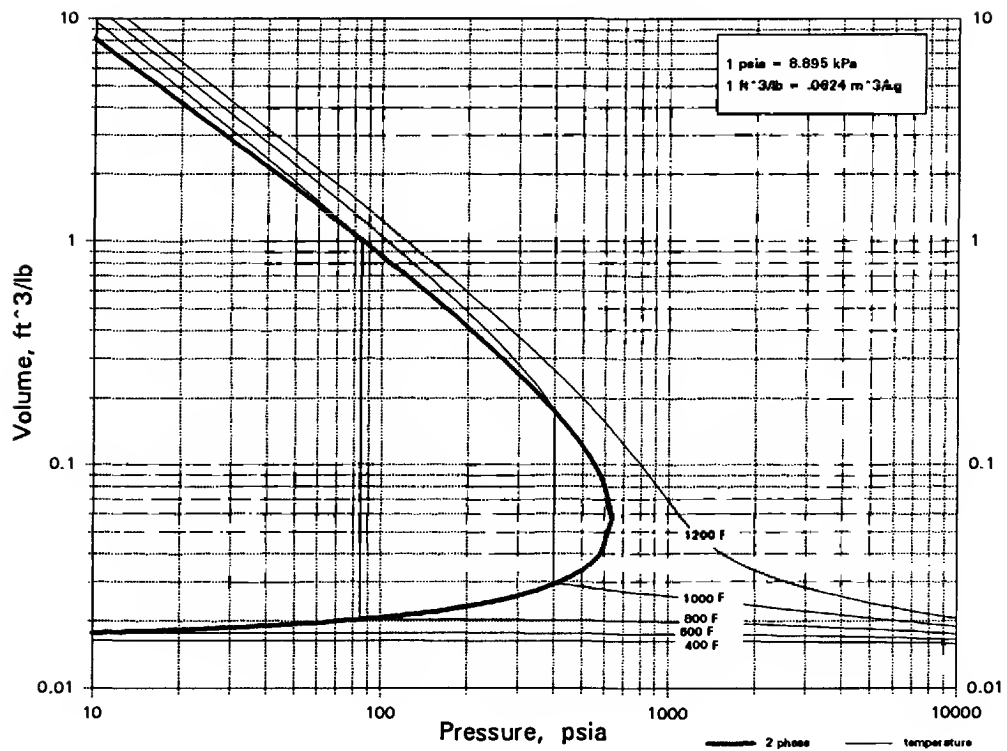
C6H6N2O2 m-NITROANILINE



C6H6N2O2 o-NITROANILINE

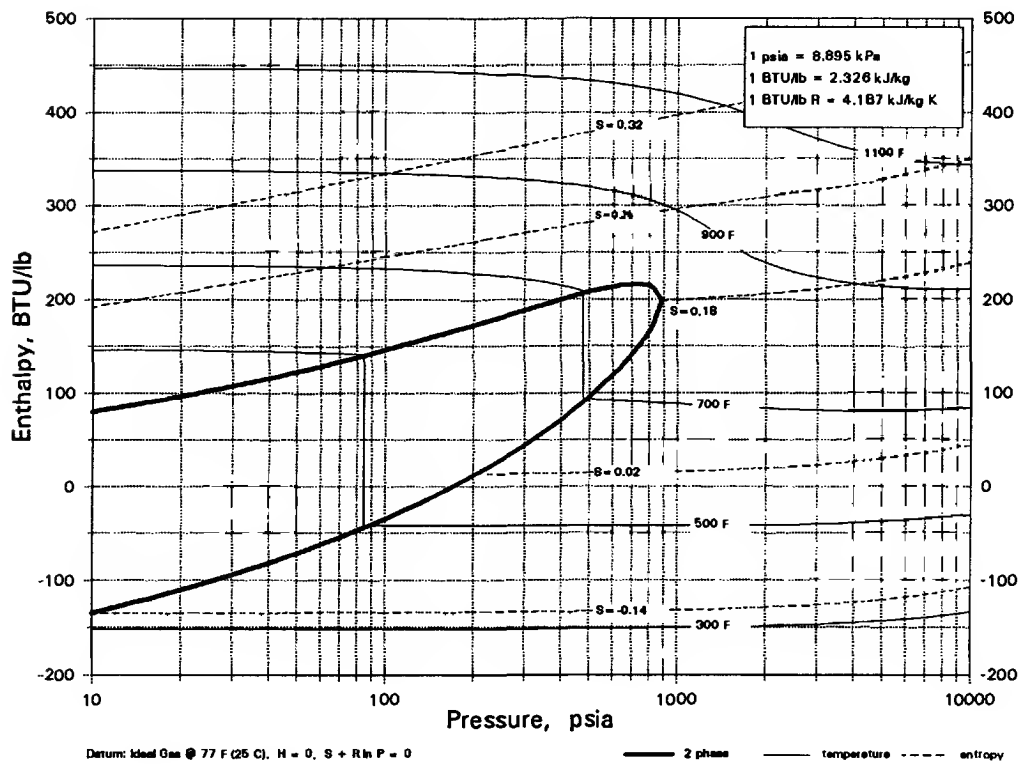
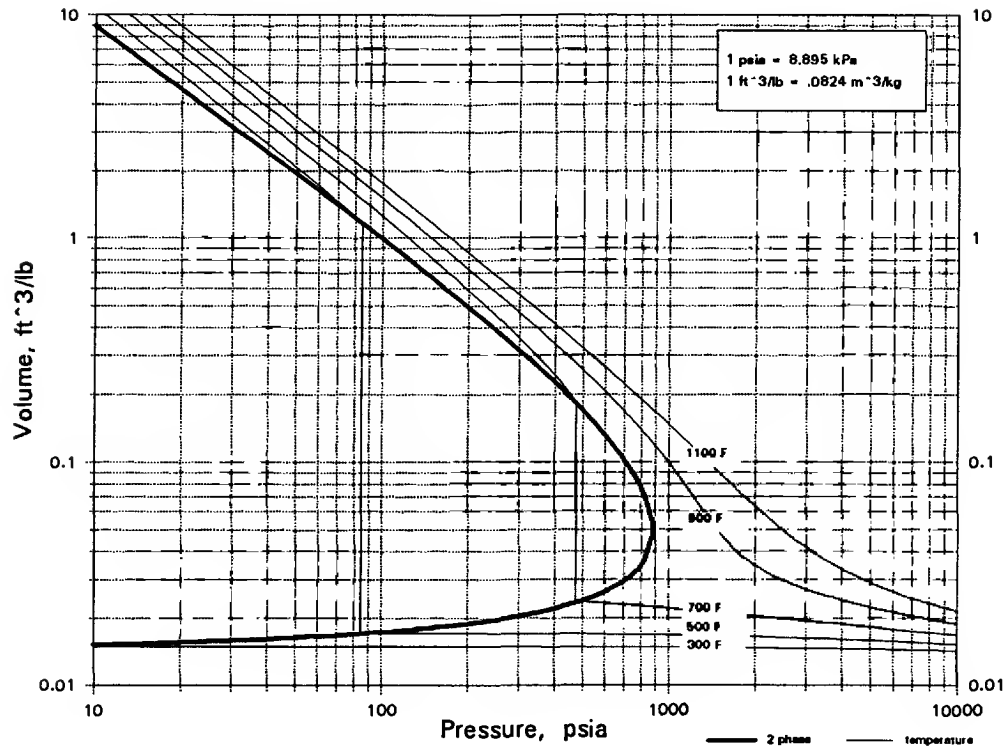


$C_6H_6N_2O_2$ p-NITROANILINE



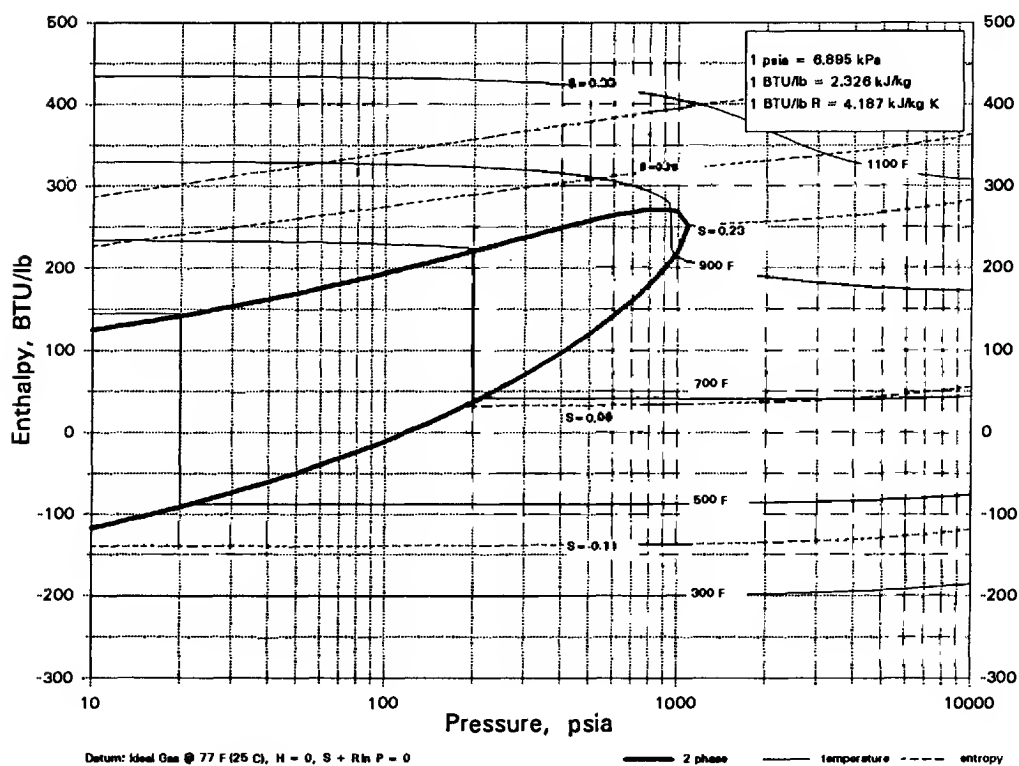
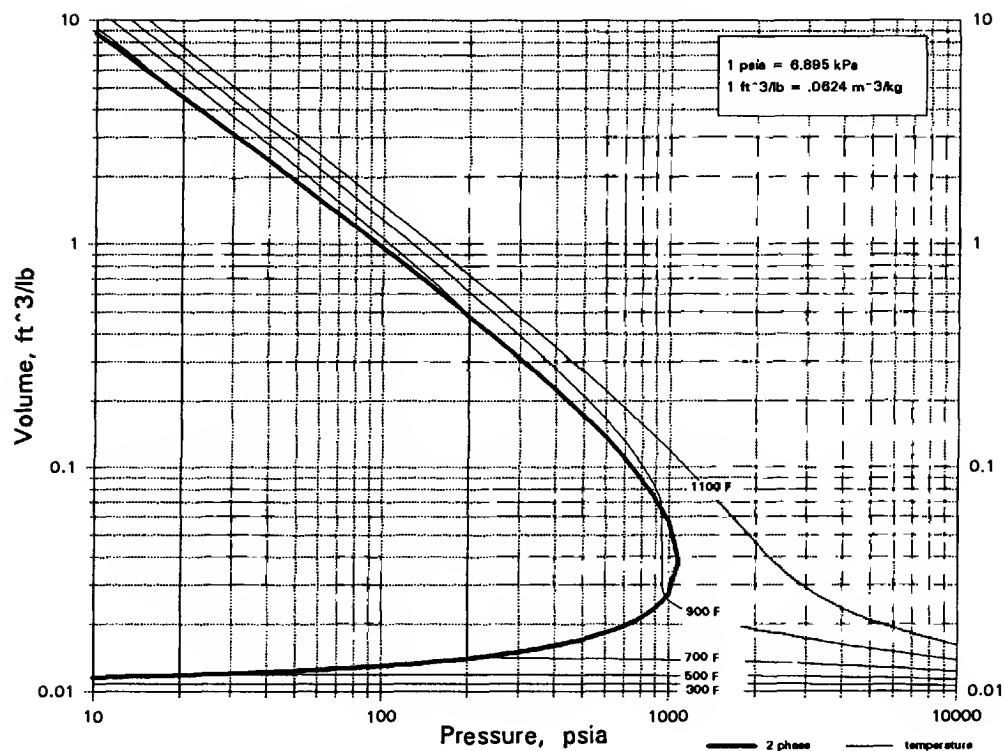
C6H6O

PHENOL



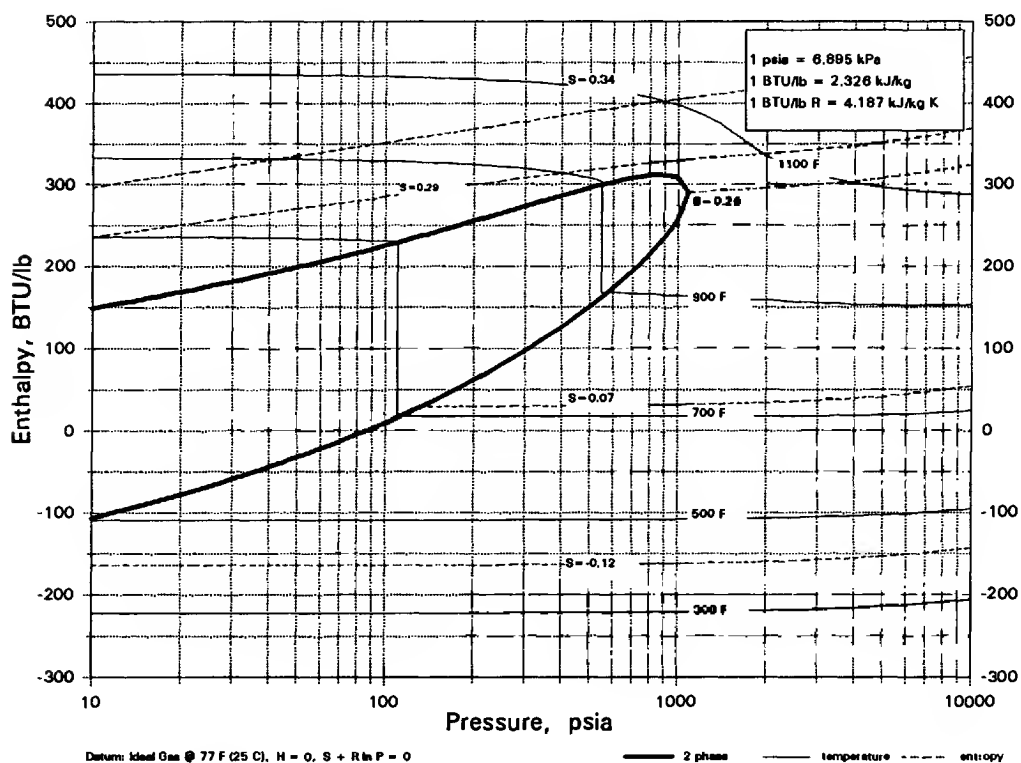
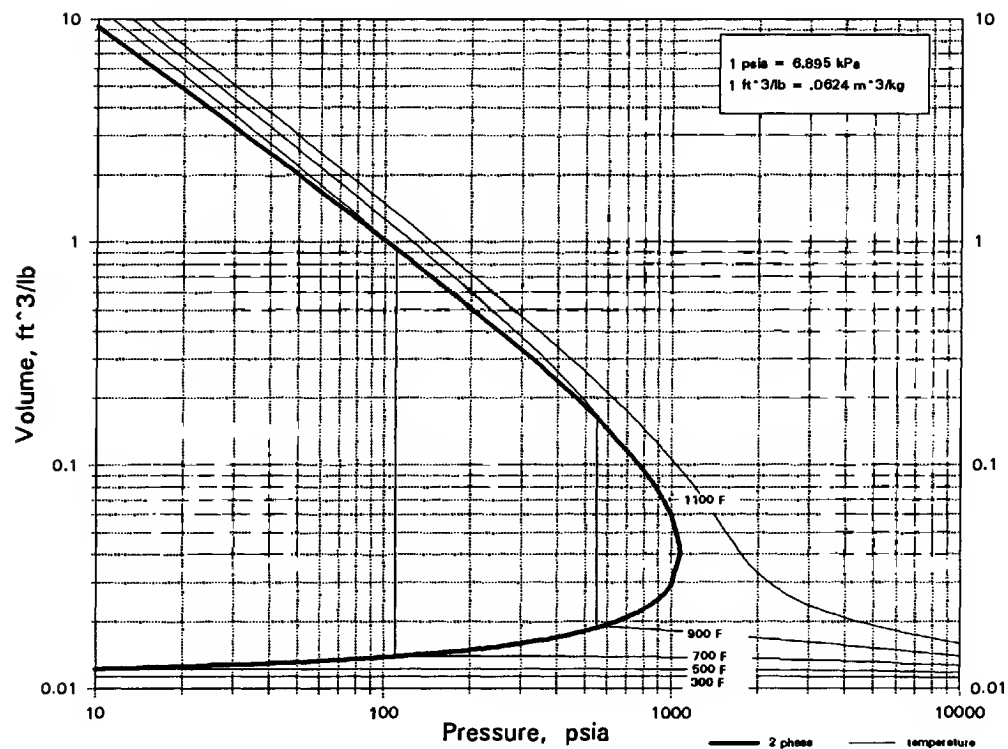
C6H6O2

1-2-BENZENEDIOL



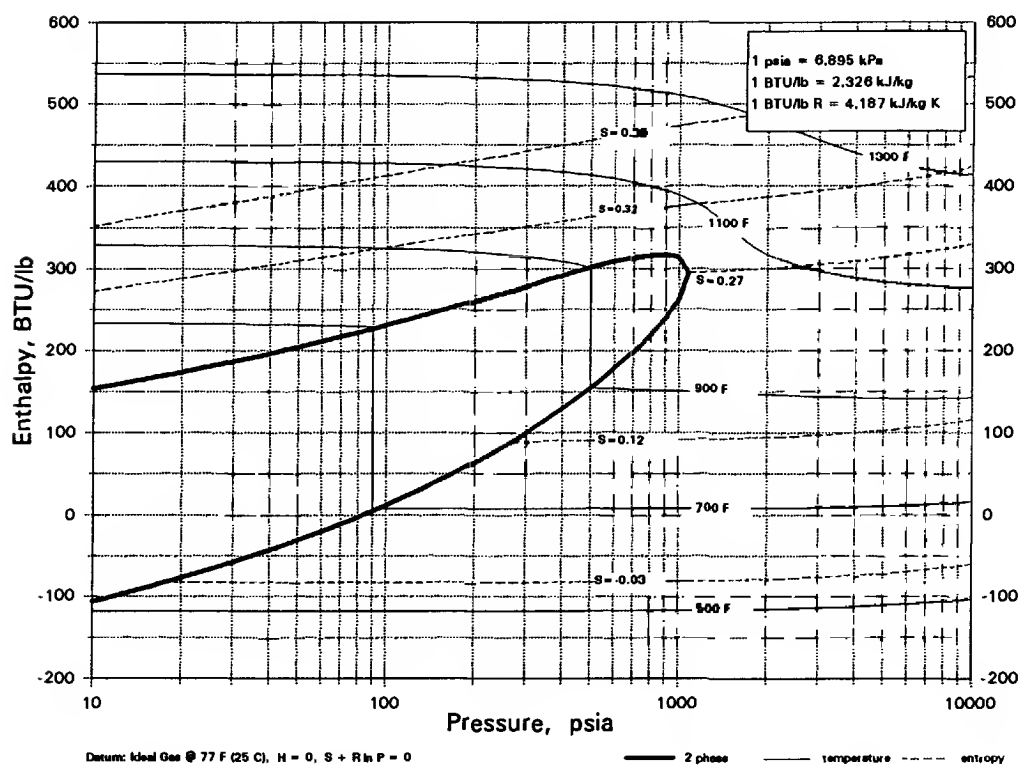
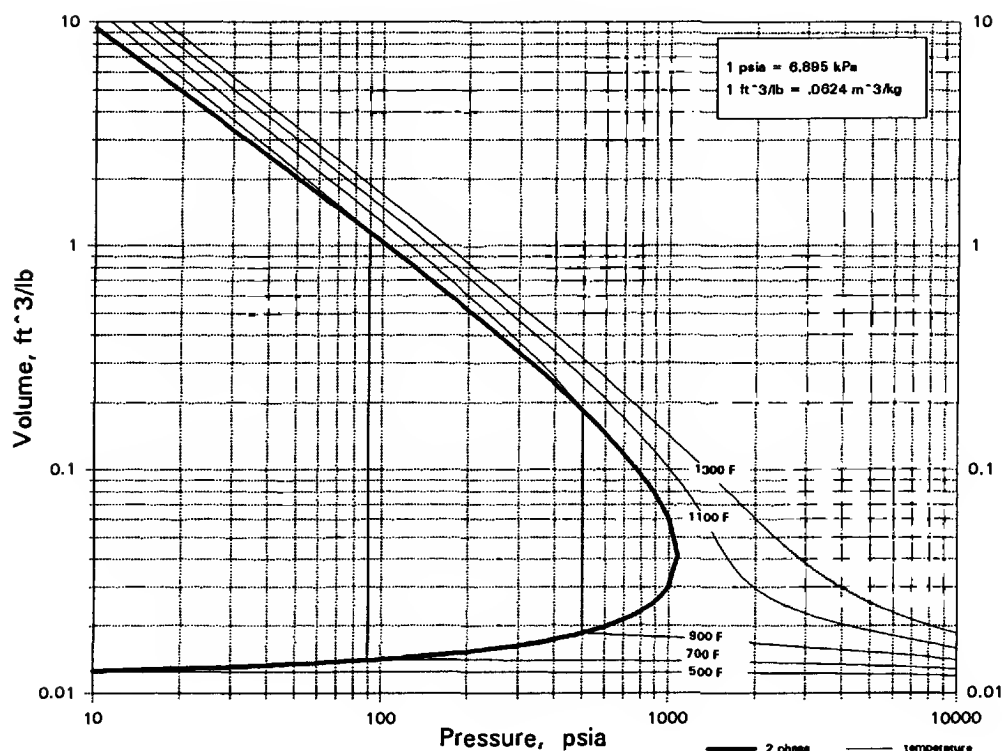
C6H6O2

1-3-BENZENEDIOL



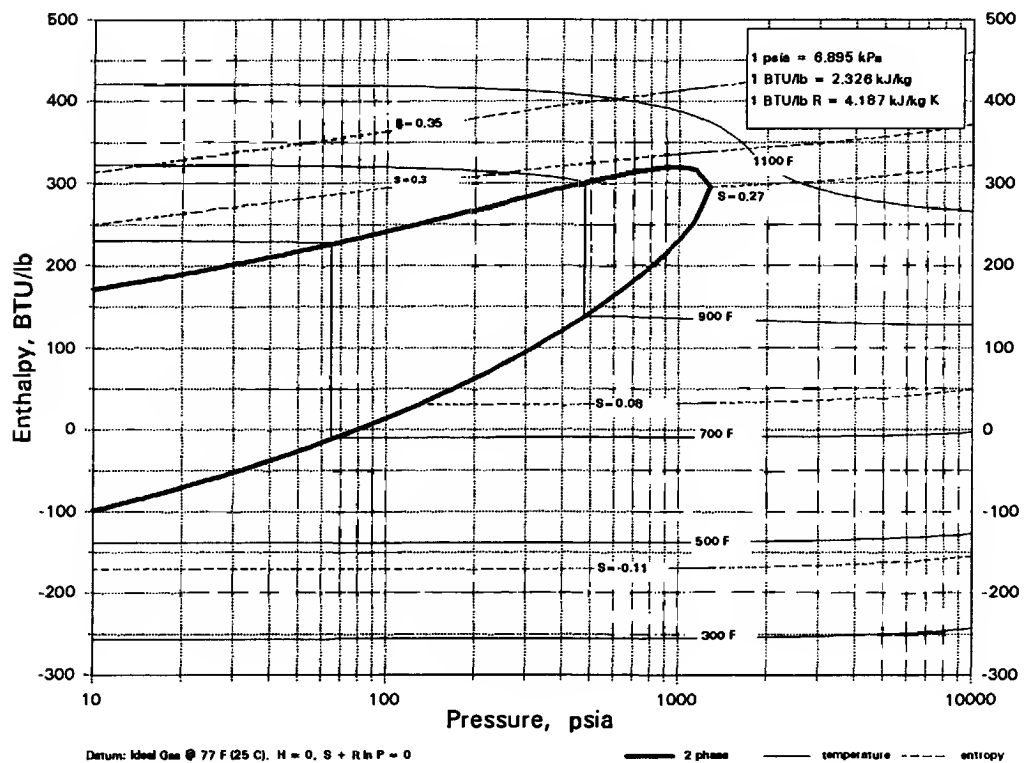
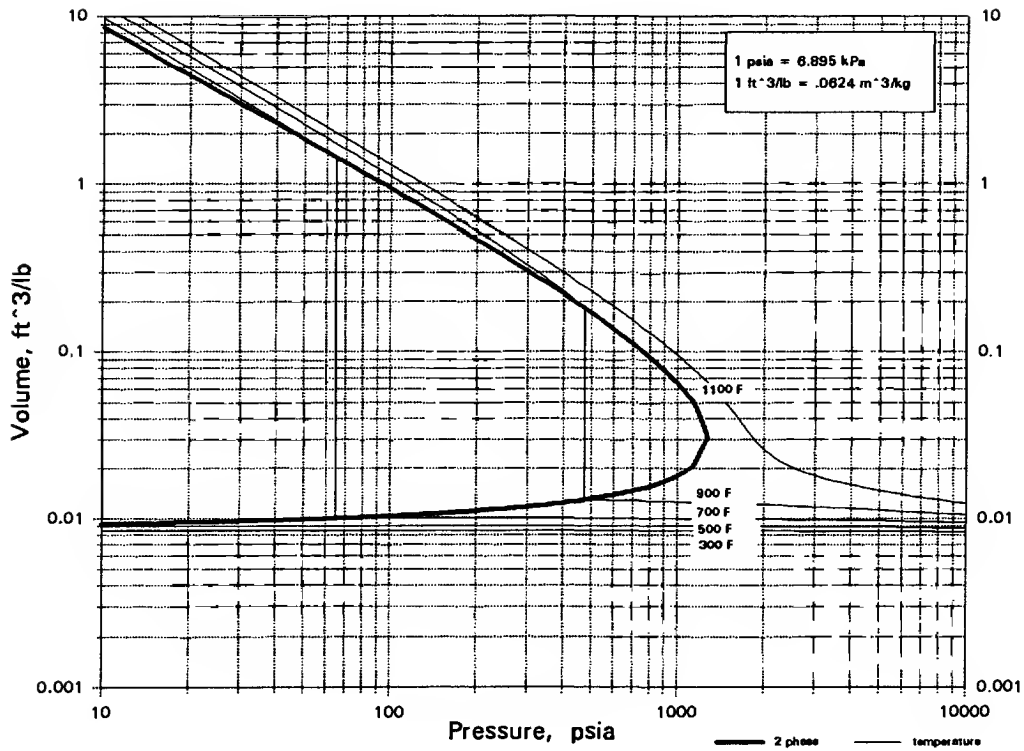
C6H6O2

p-HYDROQUINONE



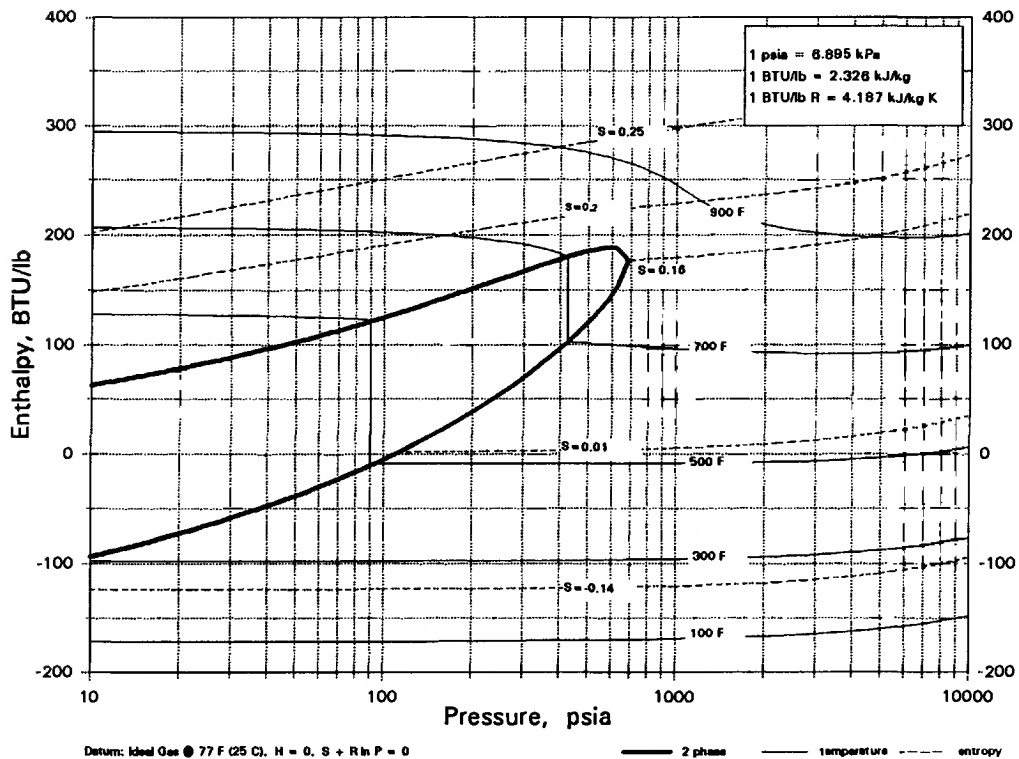
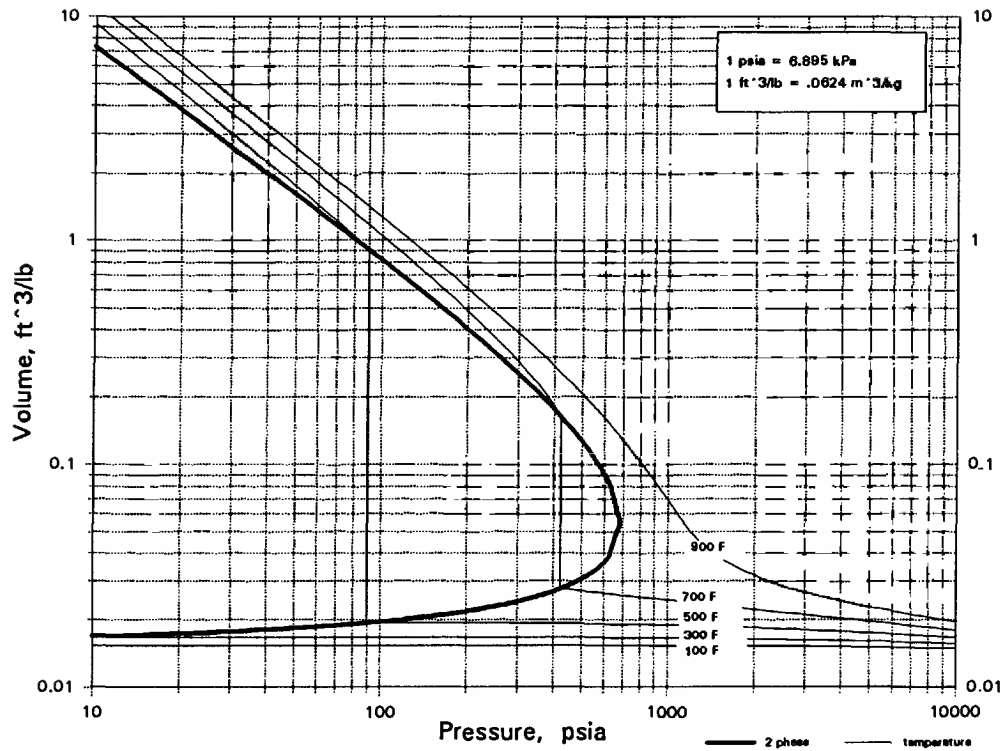
C6H6O3

1-2-3-BENZENETRIOL



C6H6S

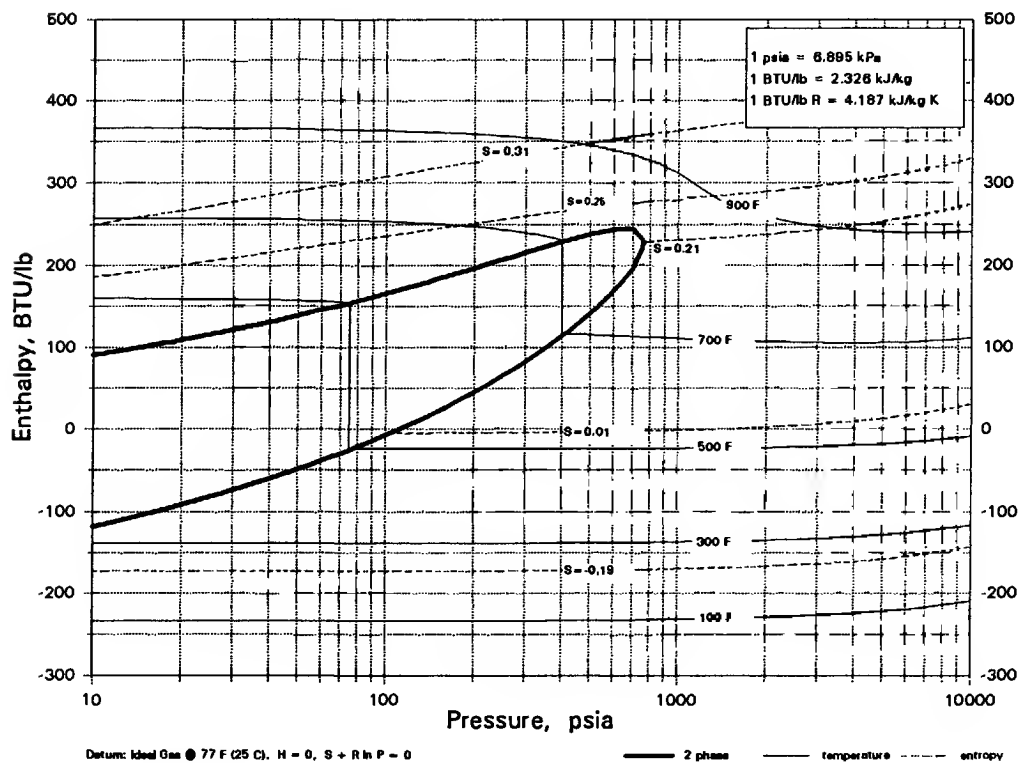
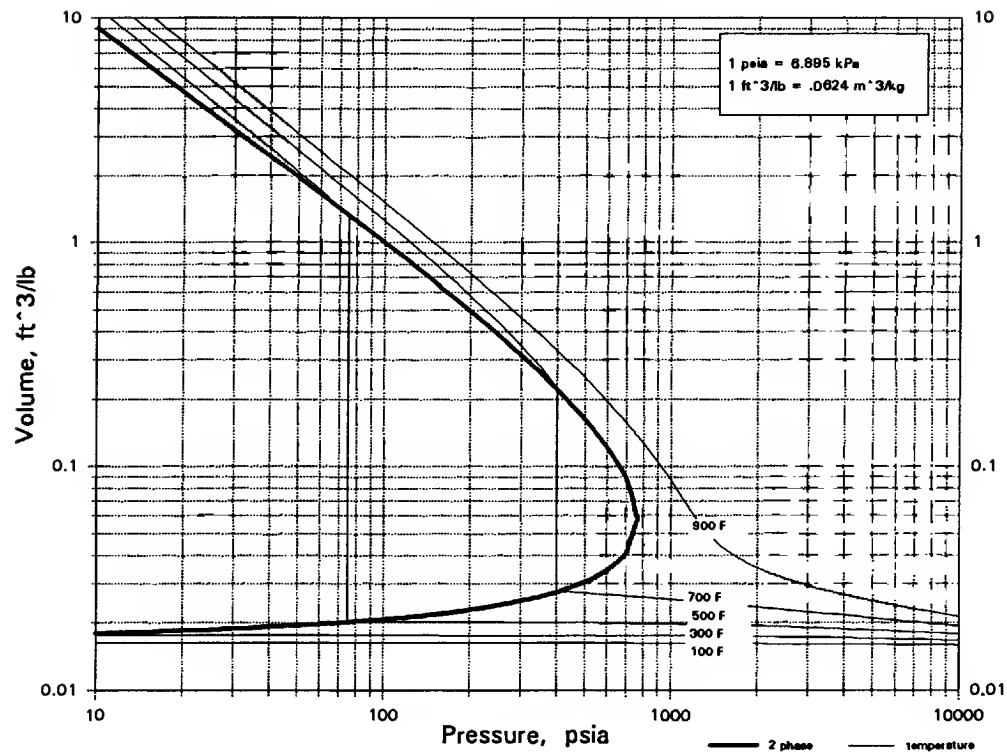
PHENYL MERCAPTAN



Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

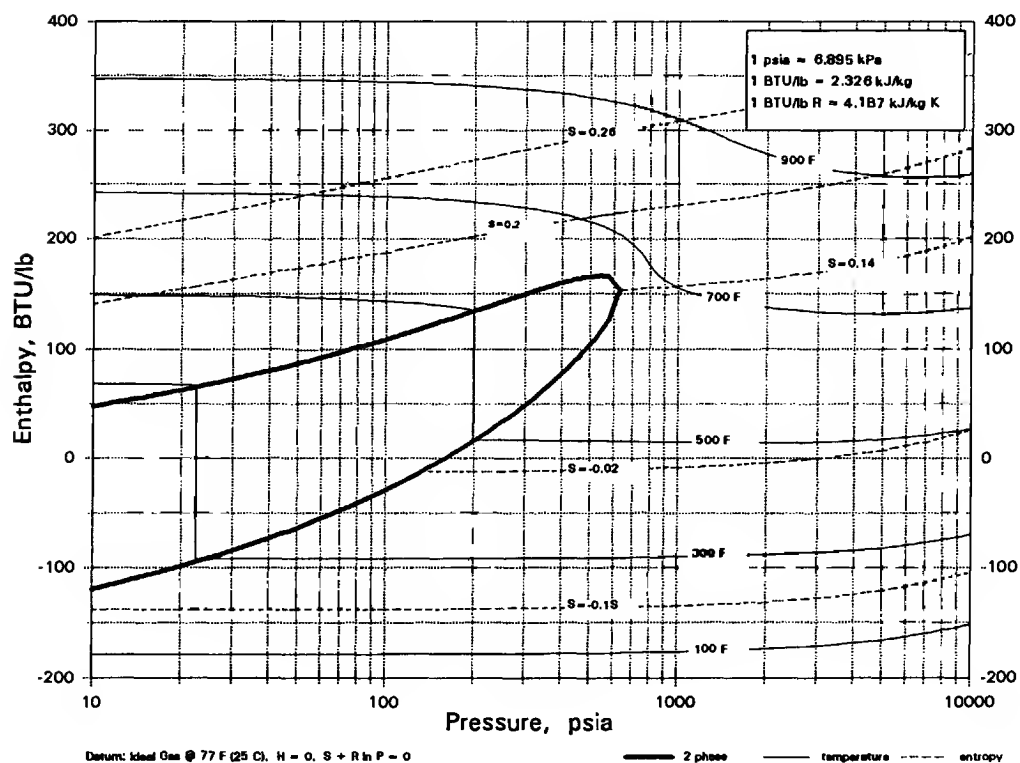
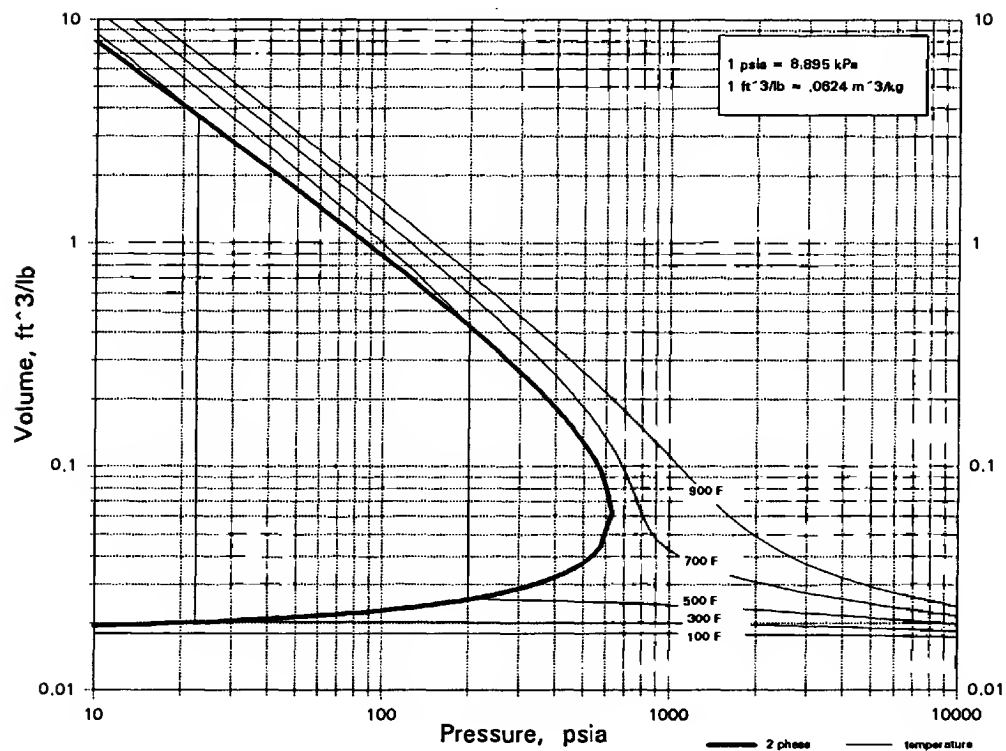
C6H7N

ANILINE



C6H7N

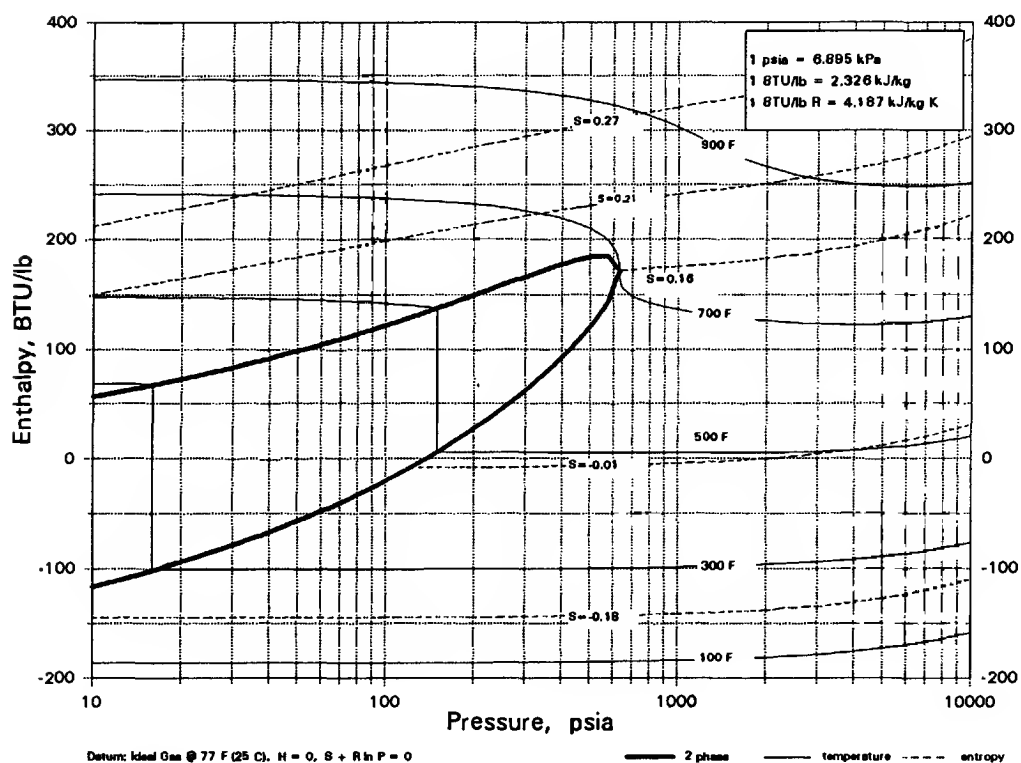
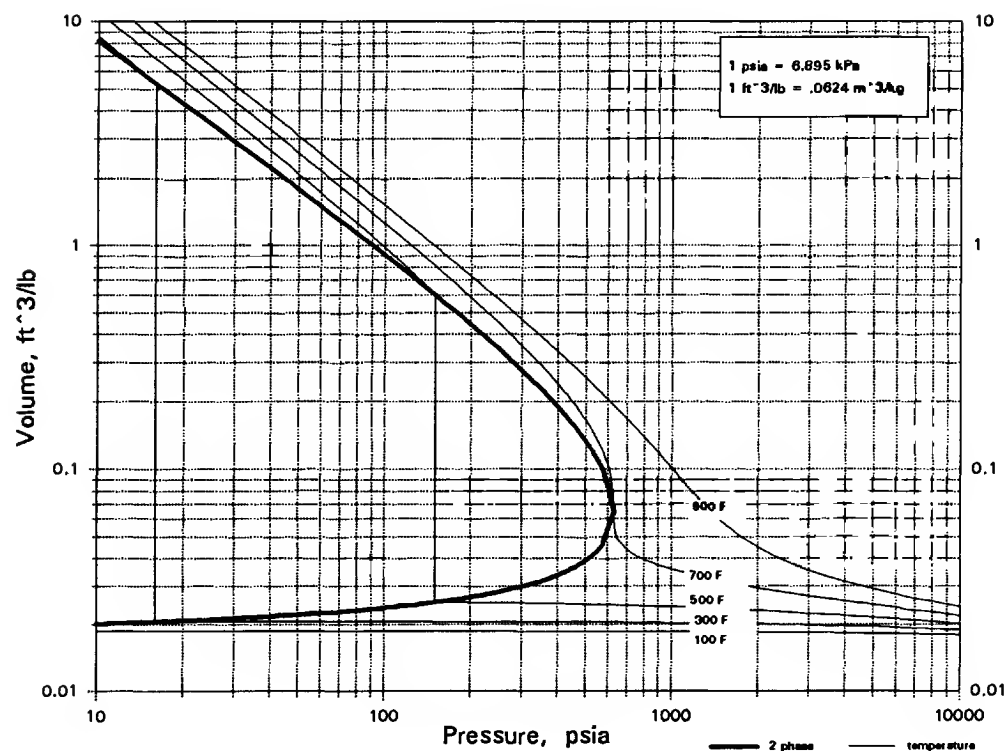
2-METHYLPYRIDINE



Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

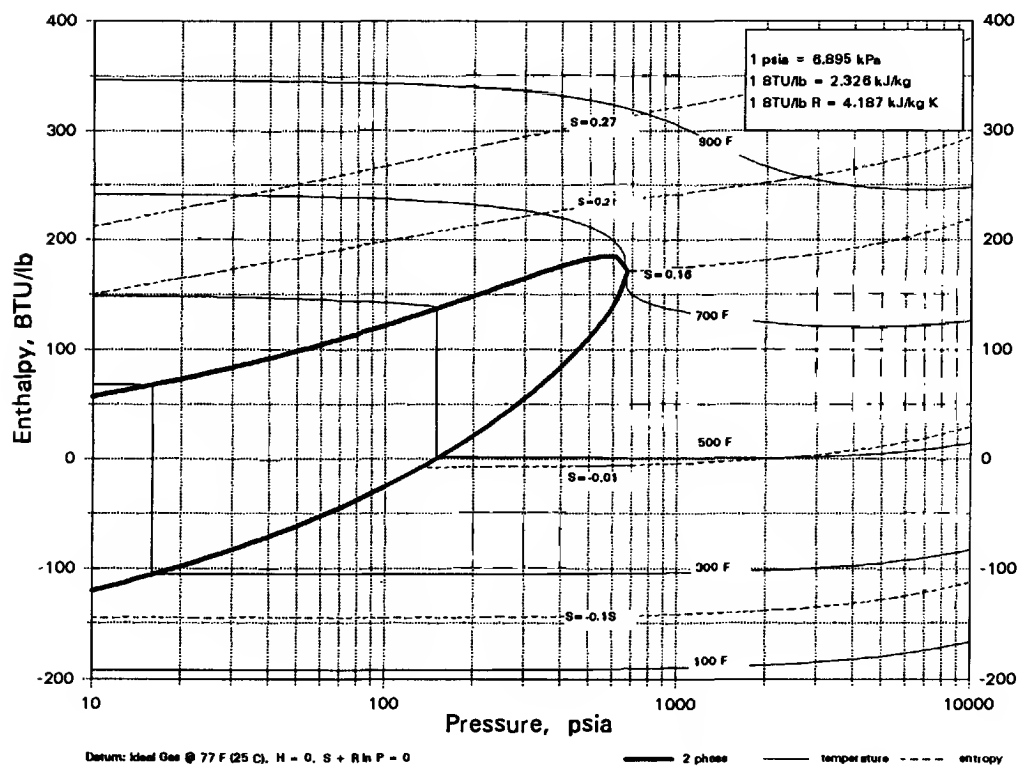
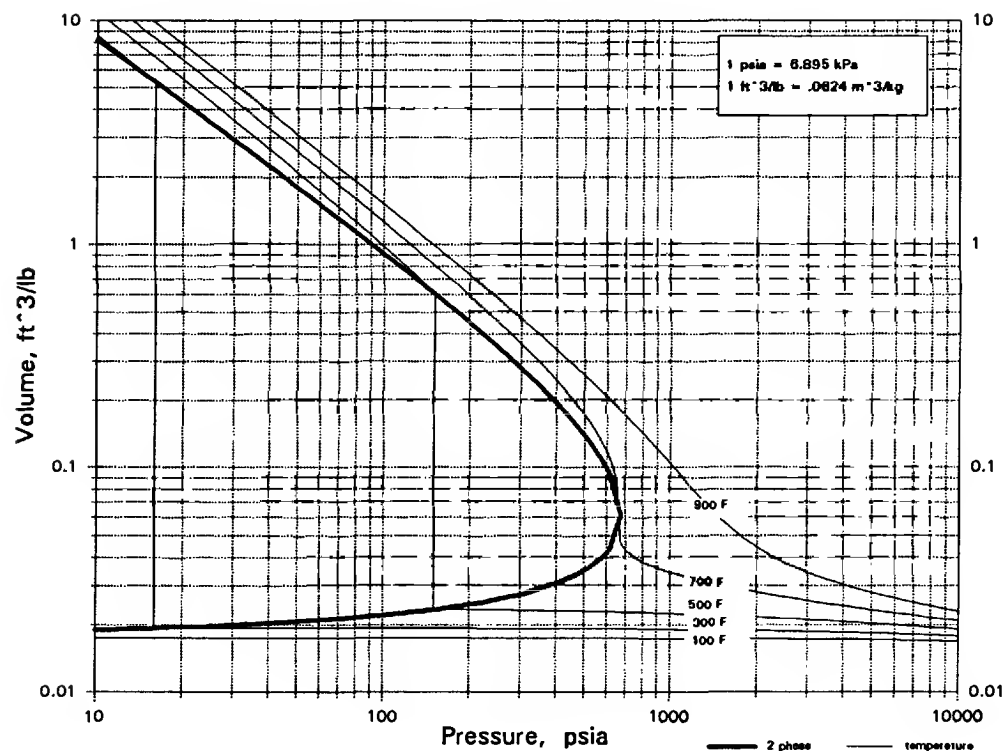
C6H7N

3-METHYLPYRIDINE



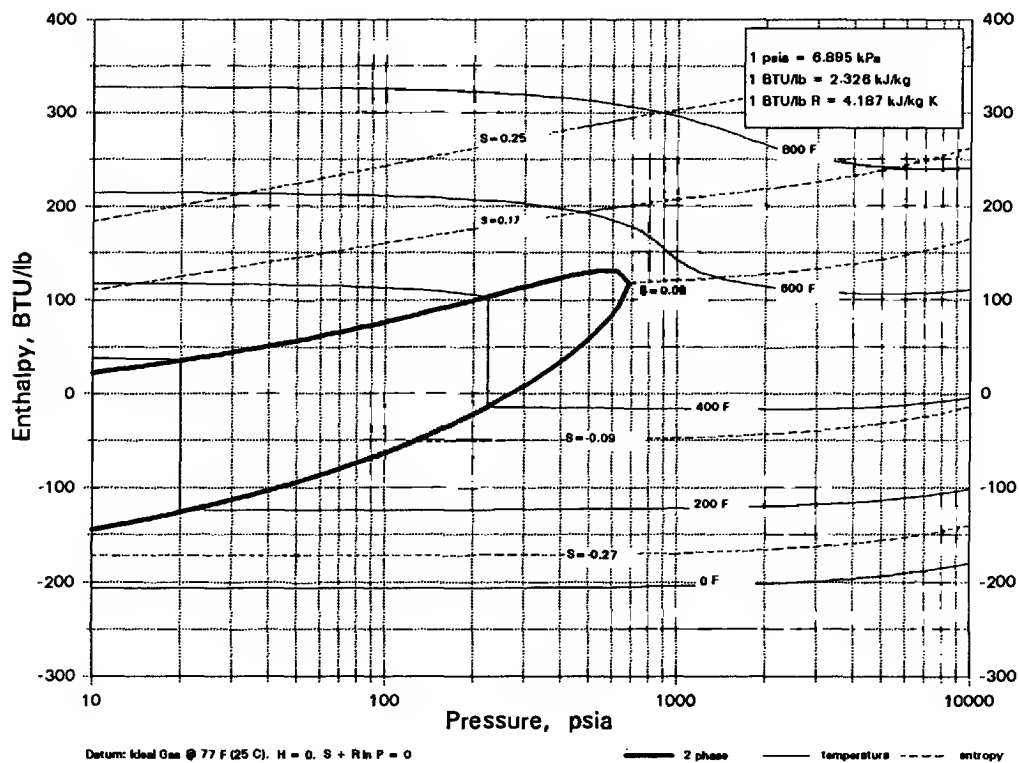
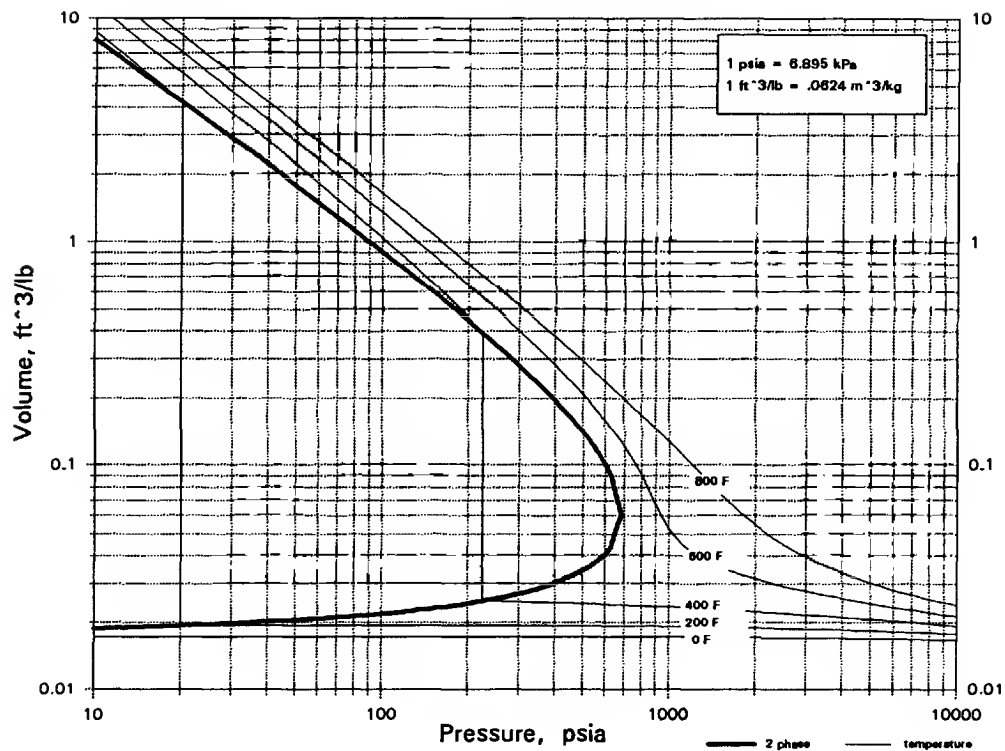
C6H7N

4-METHYLPYRIDINE



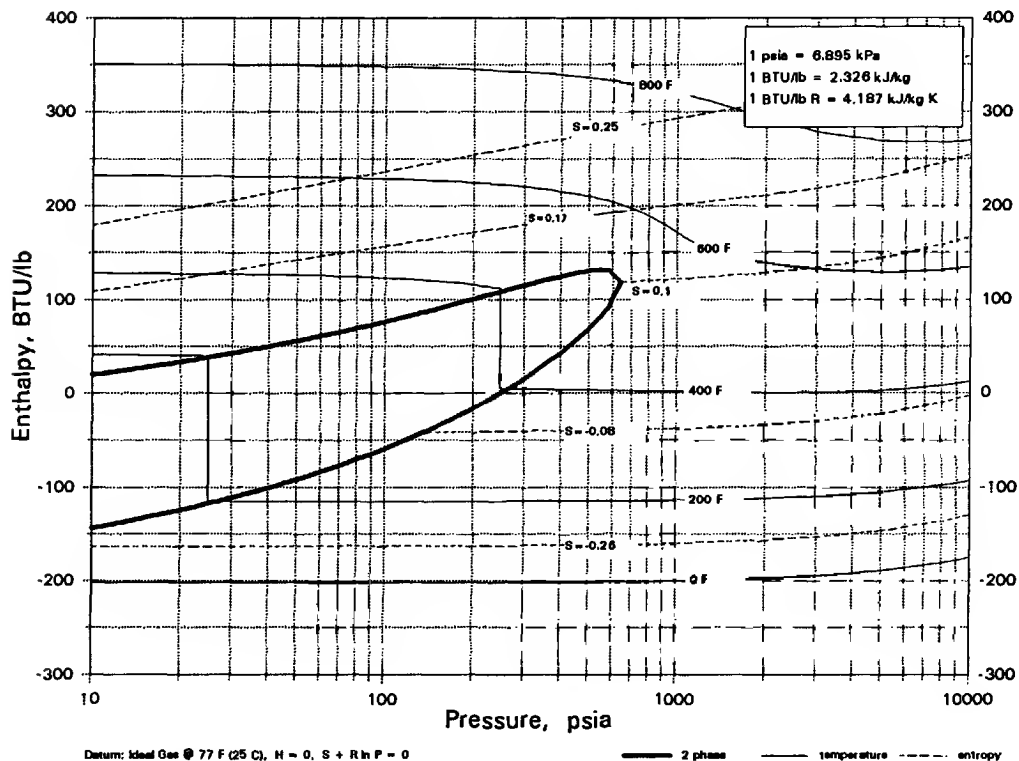
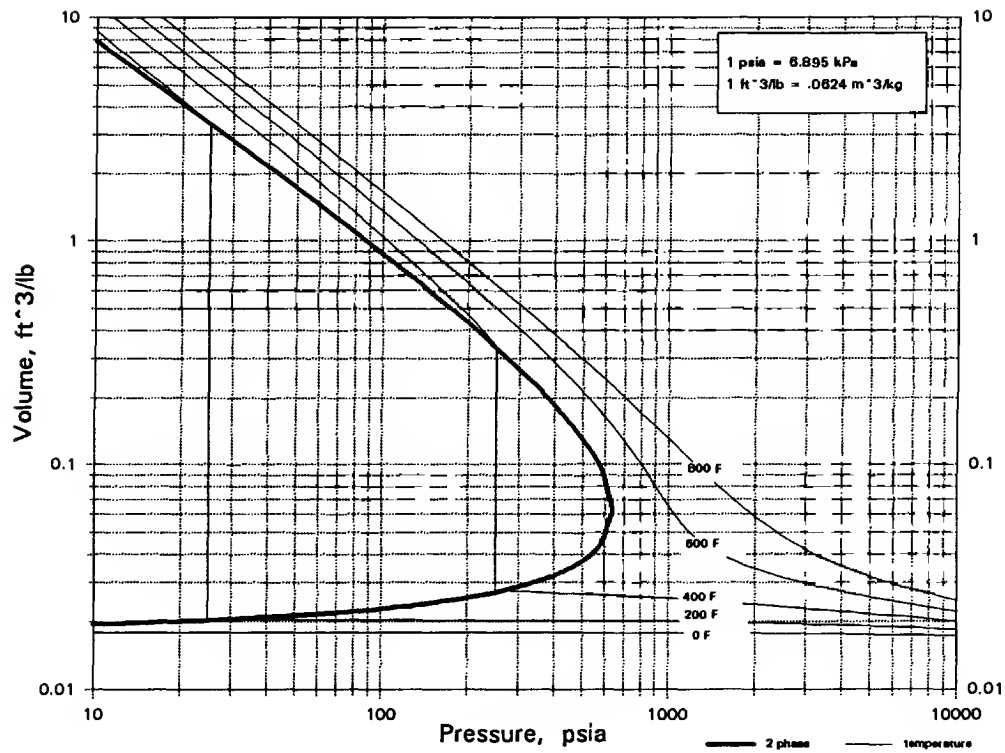
C6H8

1-3-CYCLOHEXADIENE



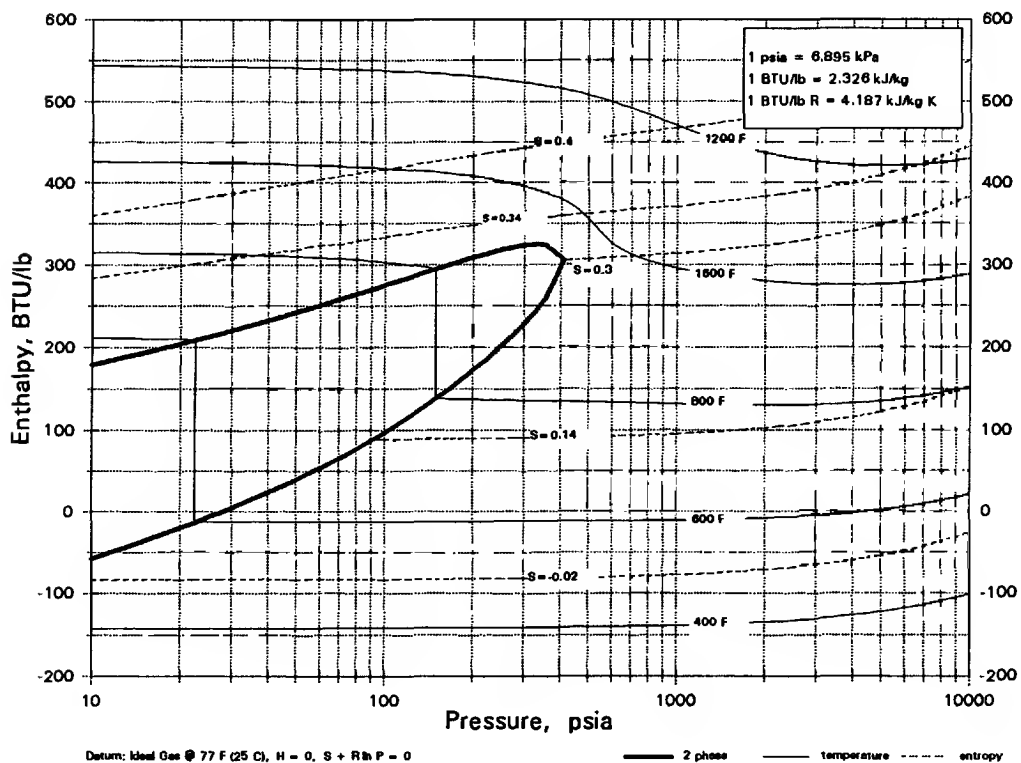
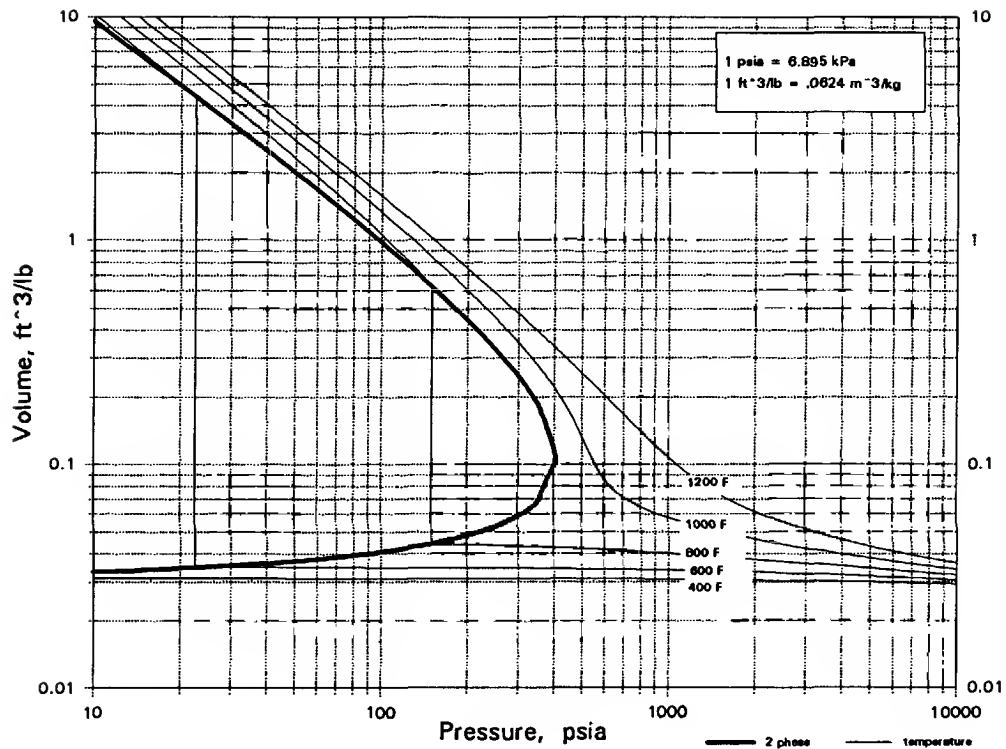
C6H8

METHYLCYCLOPENTADIENE



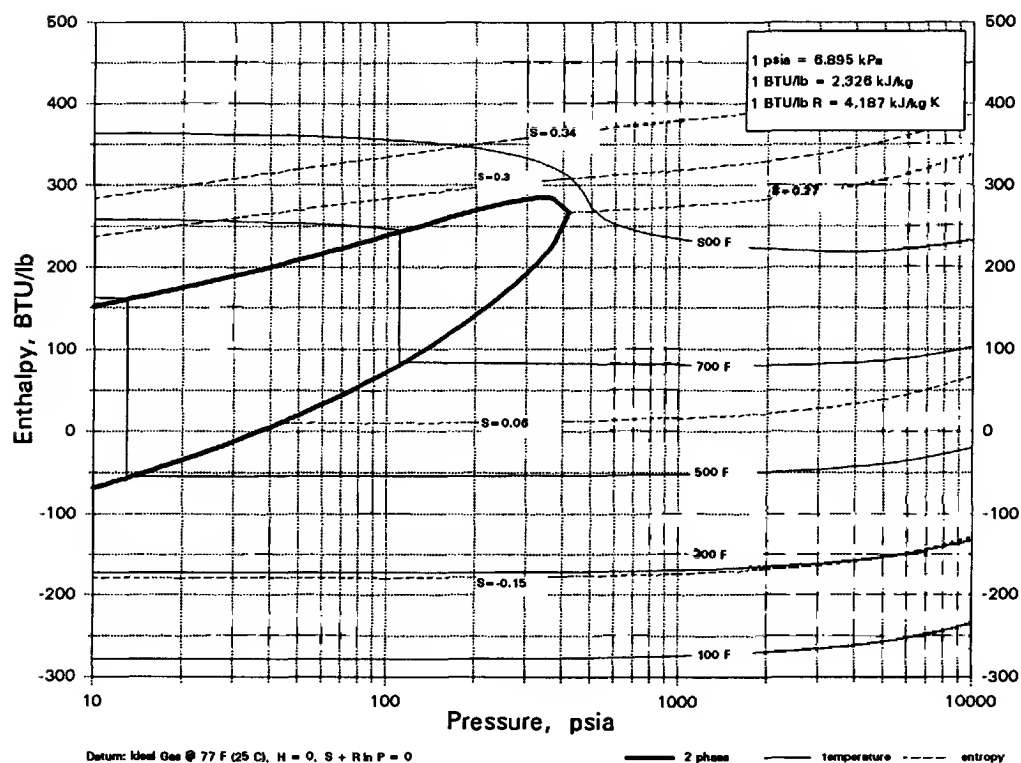
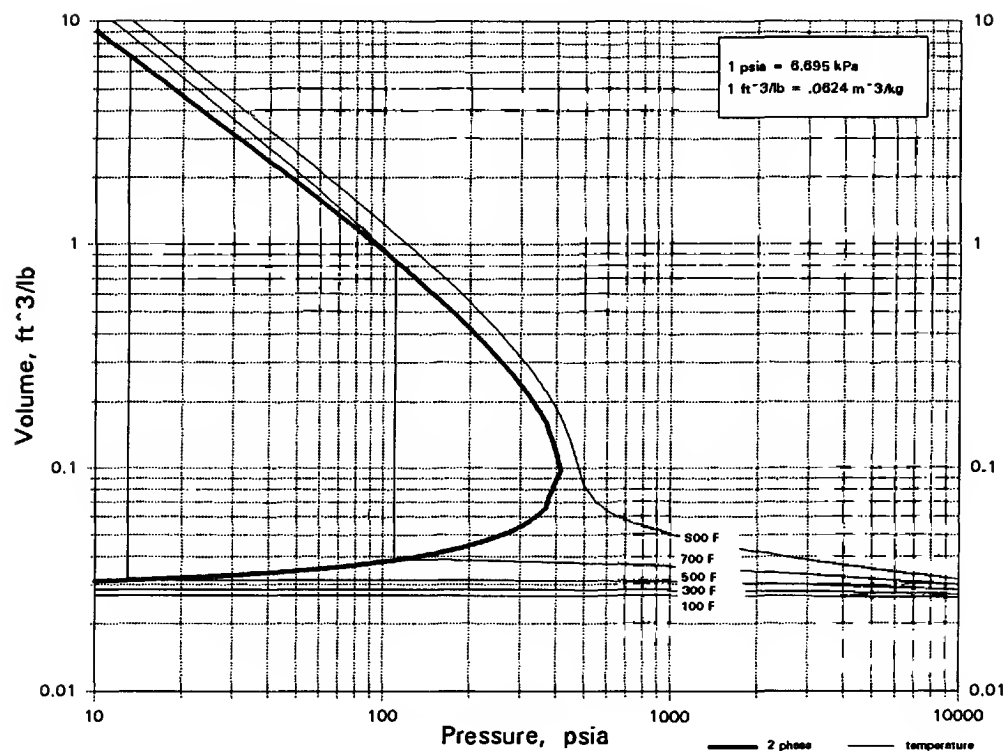
C6H8N2

ADIPONITRILE



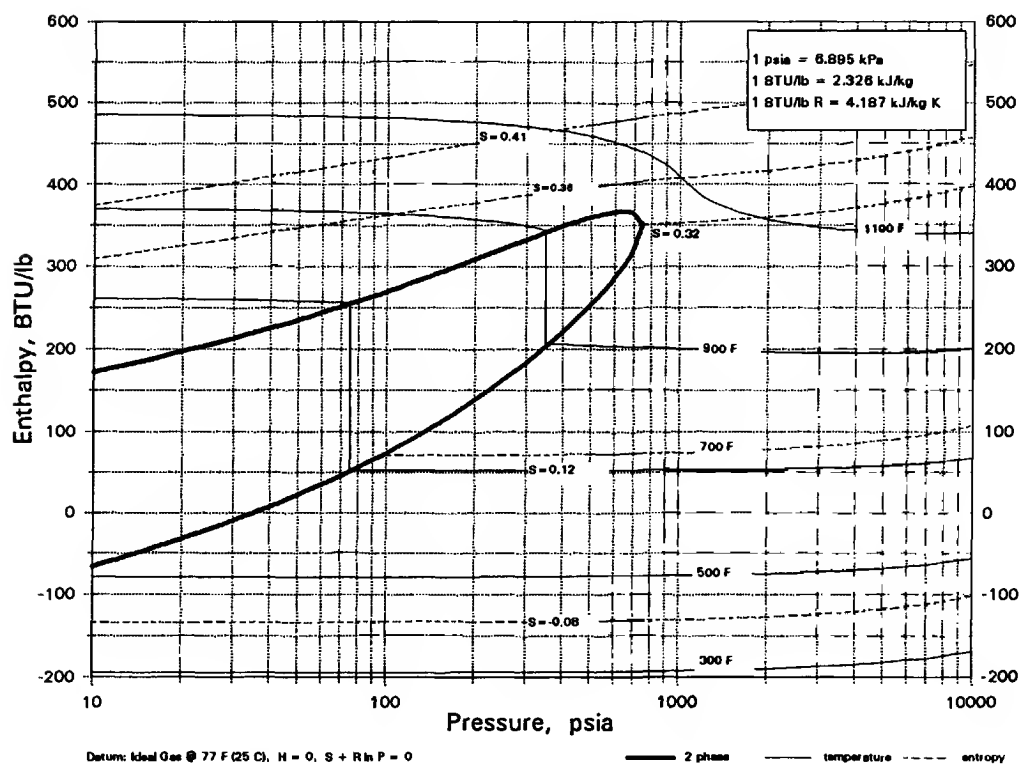
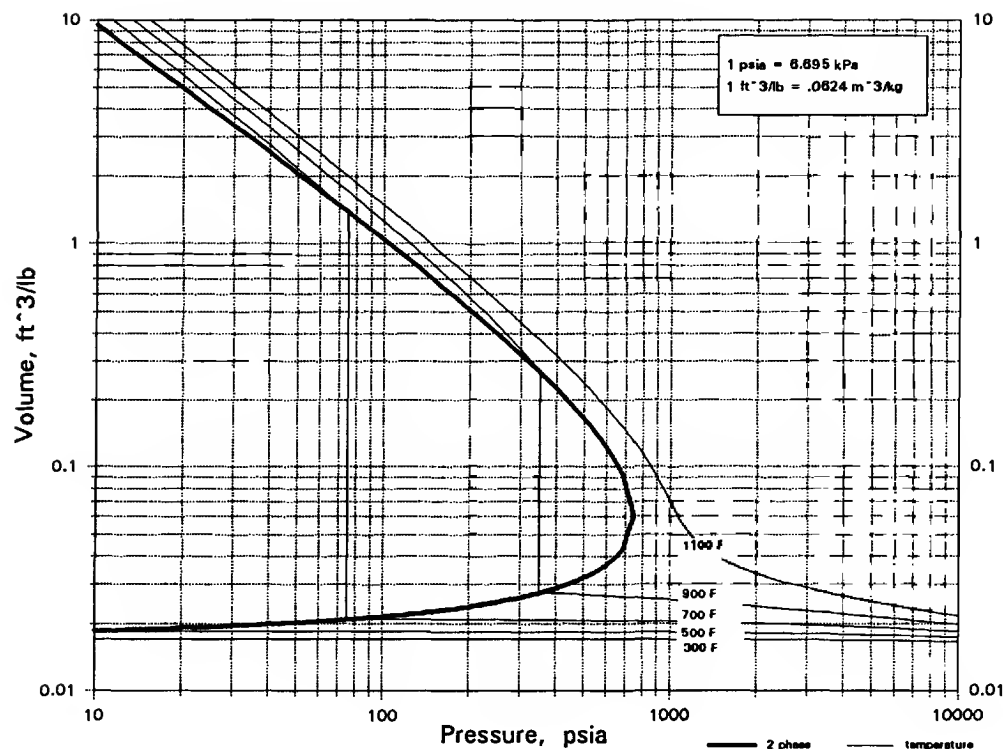
C6H8N2

METHYLGLUTARONITRILE



C6H8N2

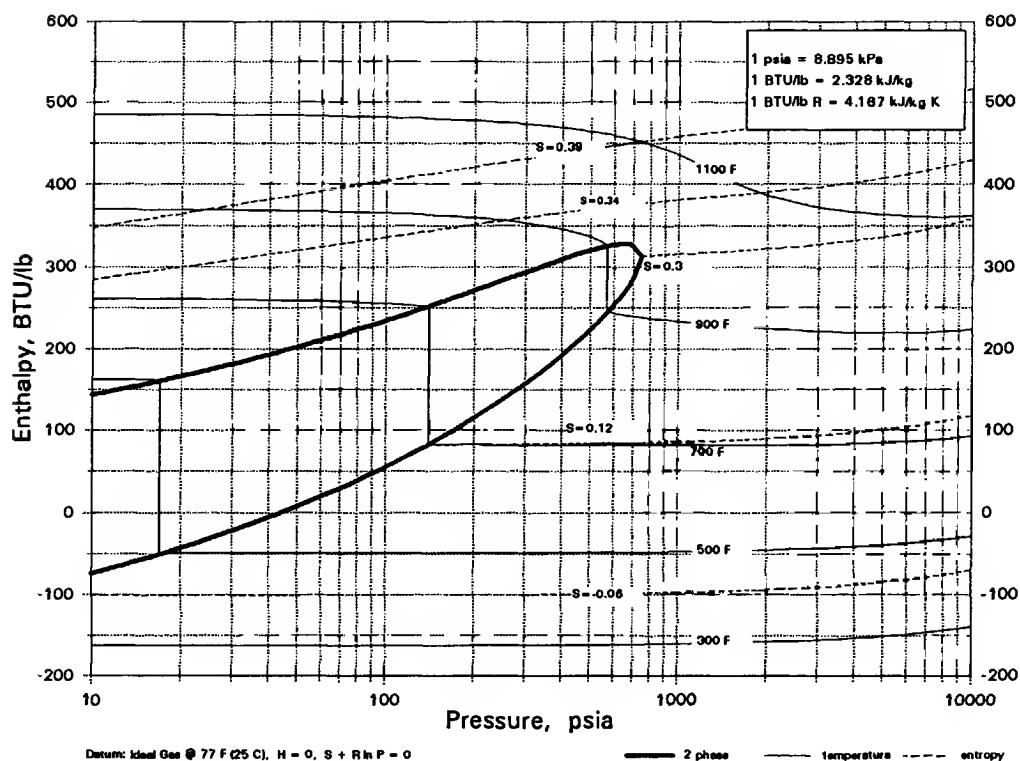
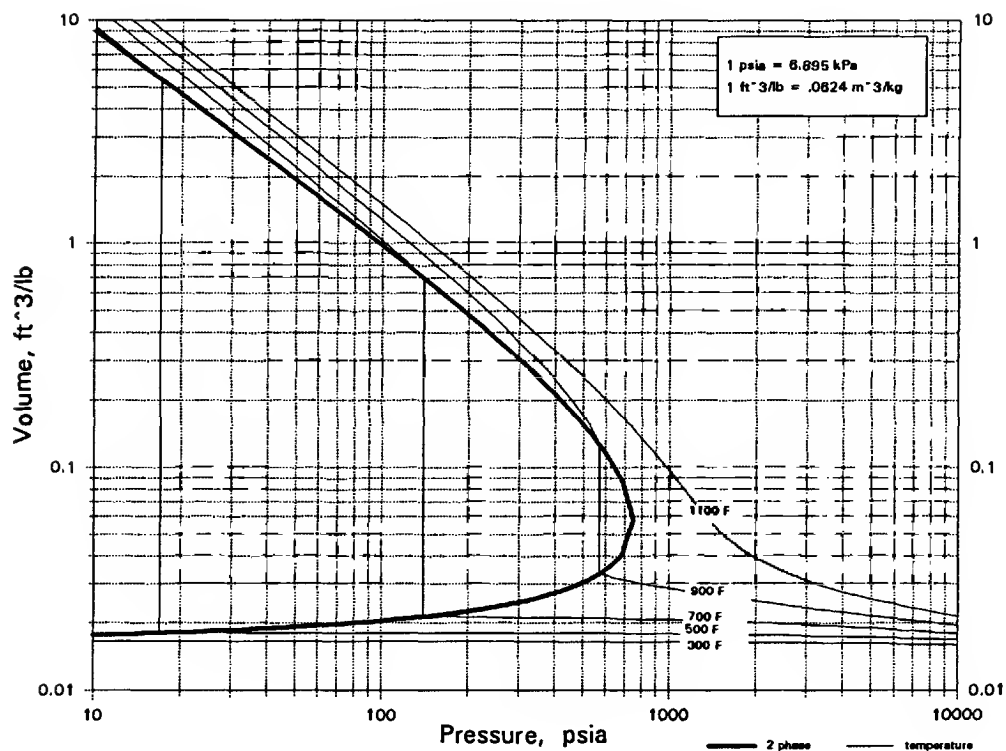
m-PHENYLENEDIAMINE



Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

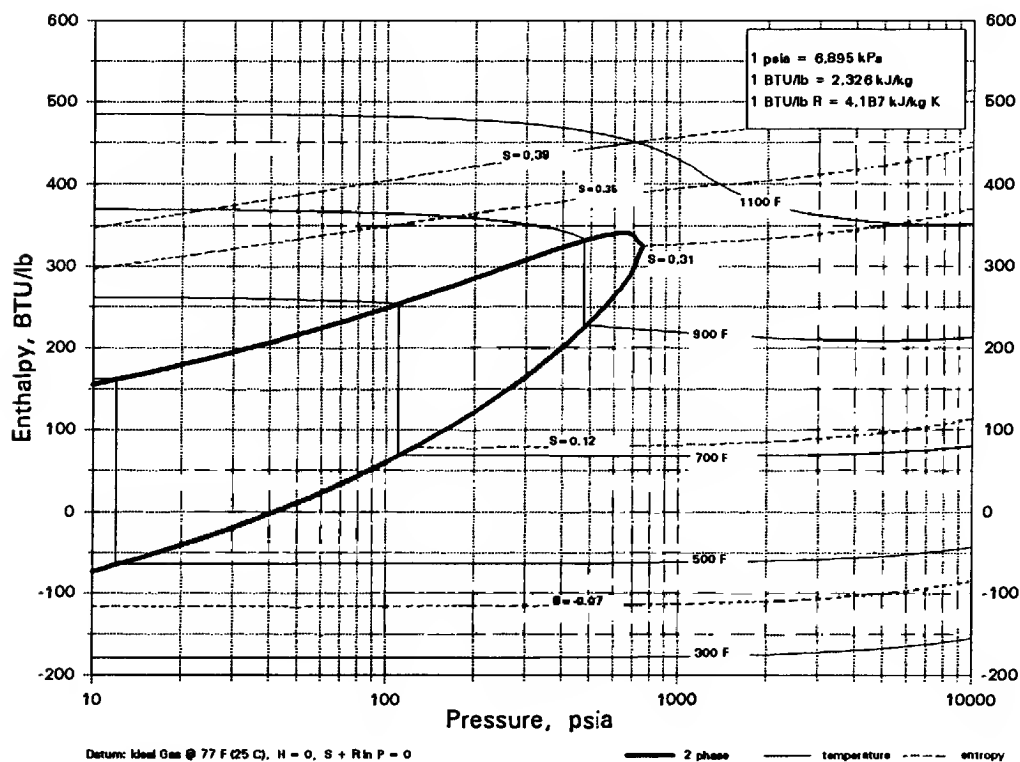
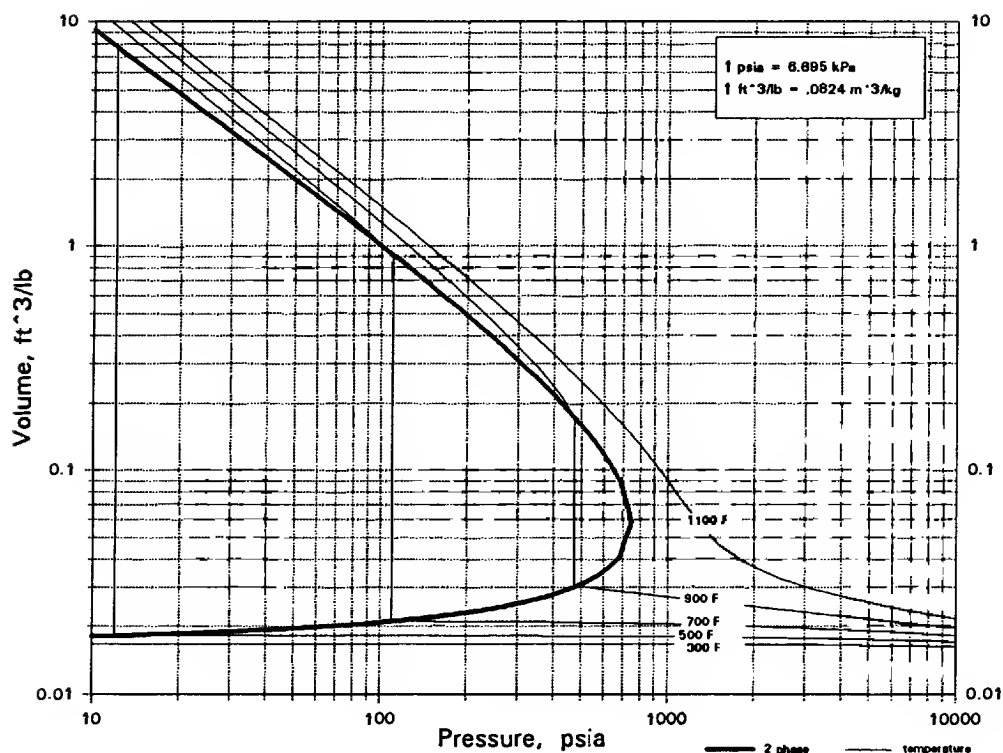
C₆H₈N₂

o-PHENYLENEDIAMINE



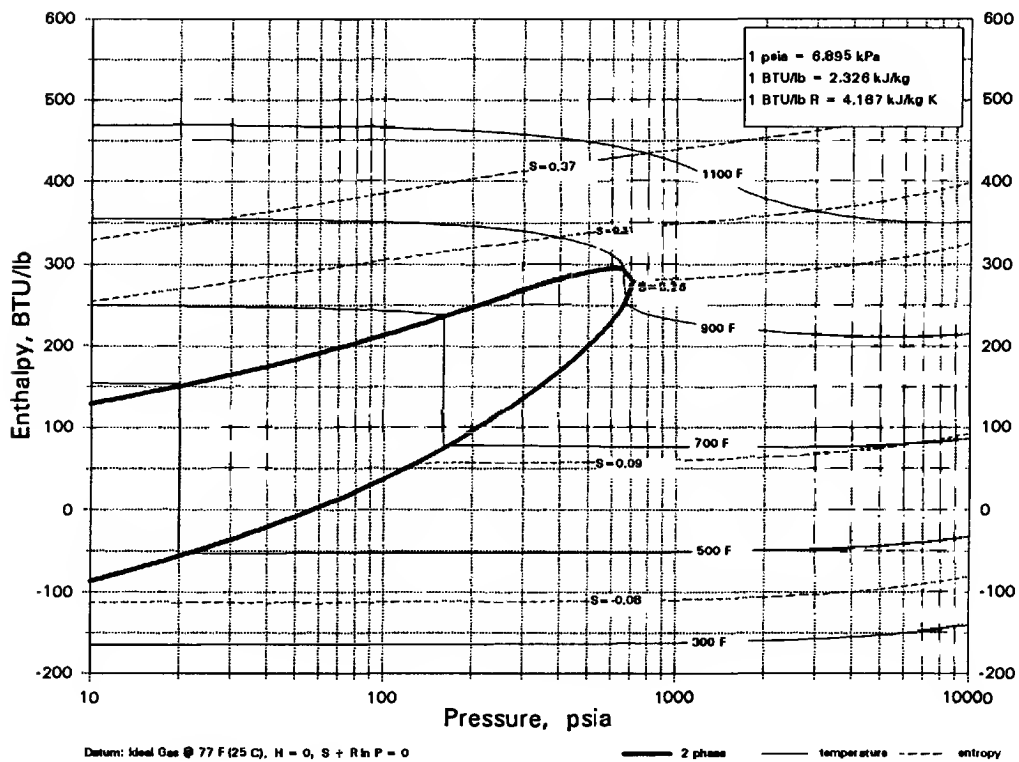
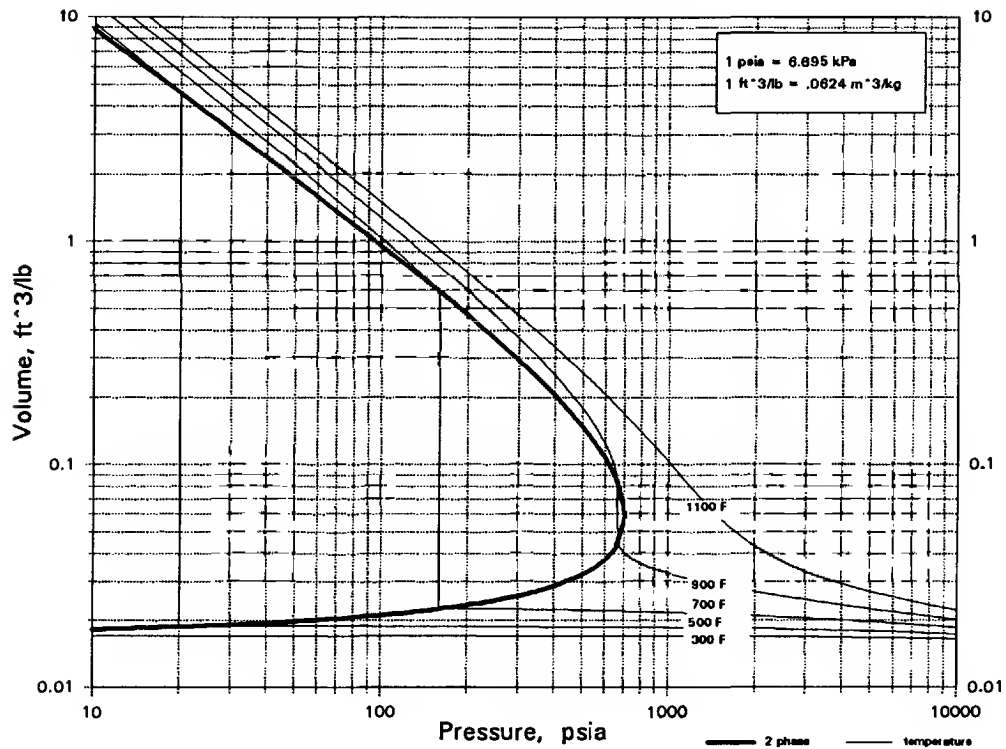
C6H8N2

p-PHENYLENEDIAMINE



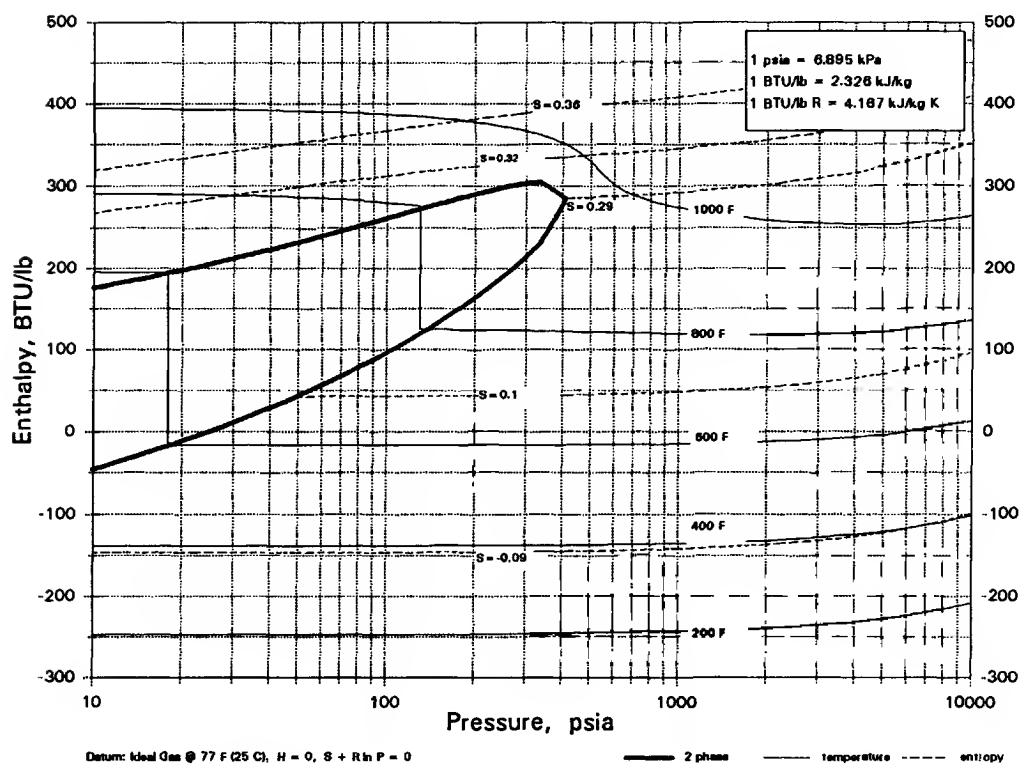
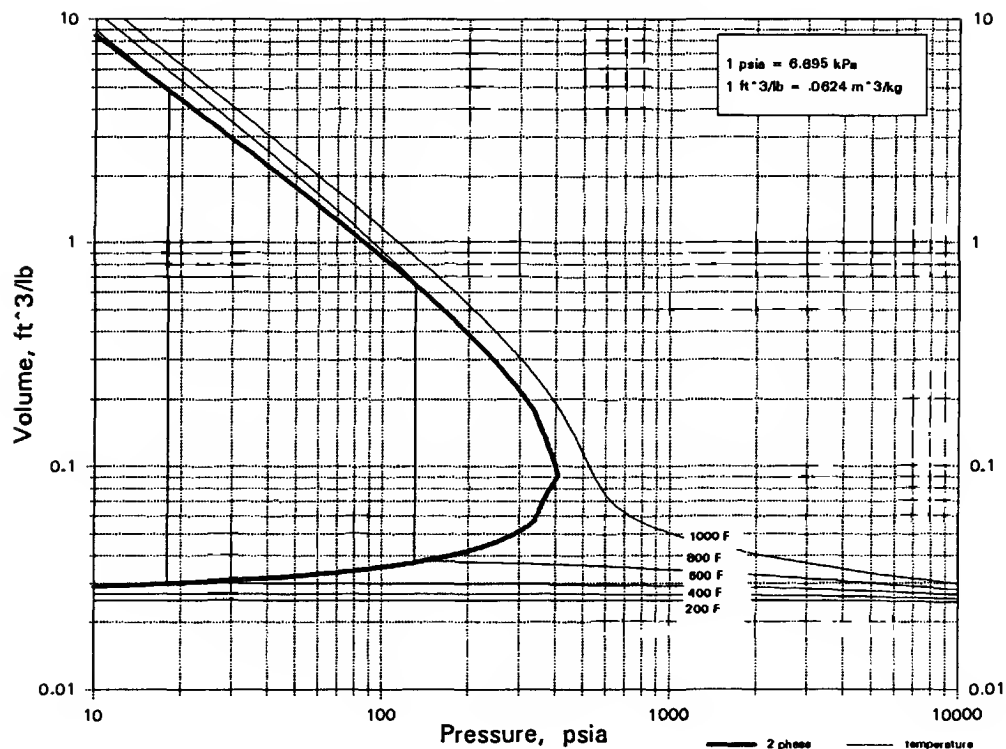
C6H8N2

PHENYLHYDRAZINE



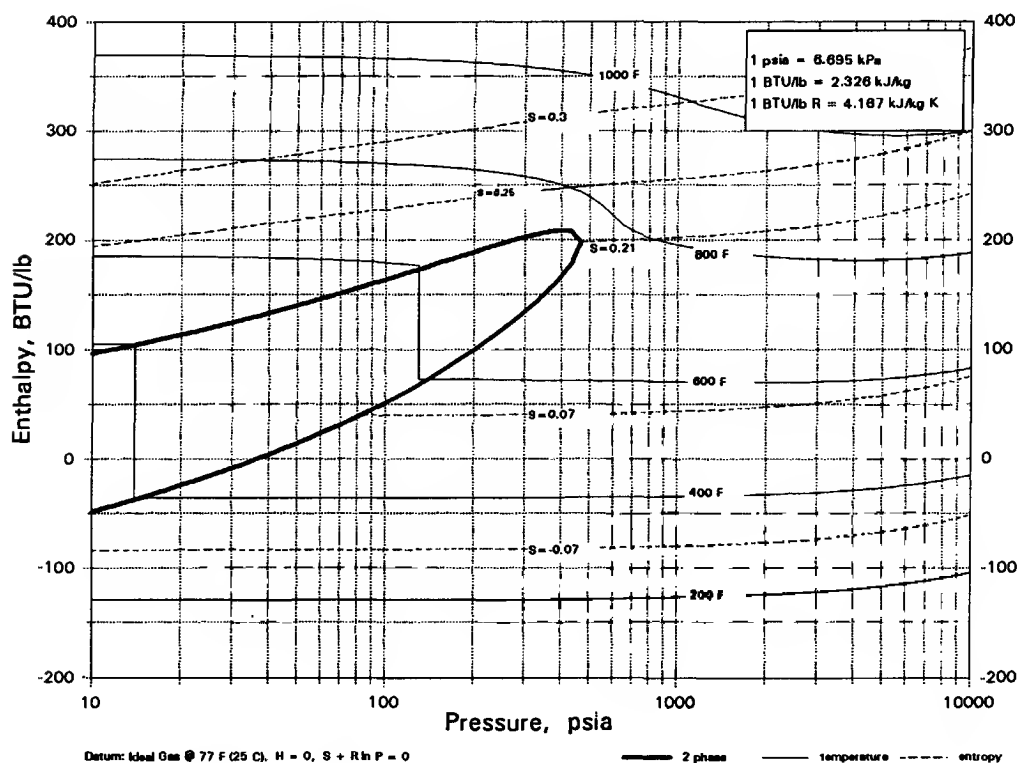
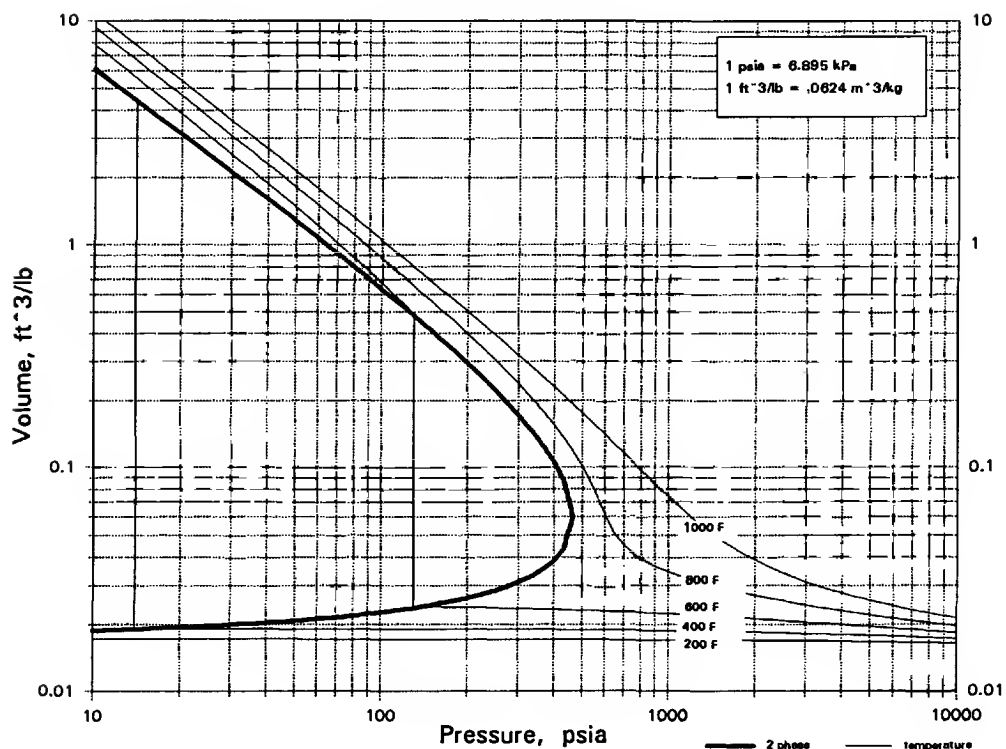
C6H8N2O

BIS(CYANOETHYL)ETHER



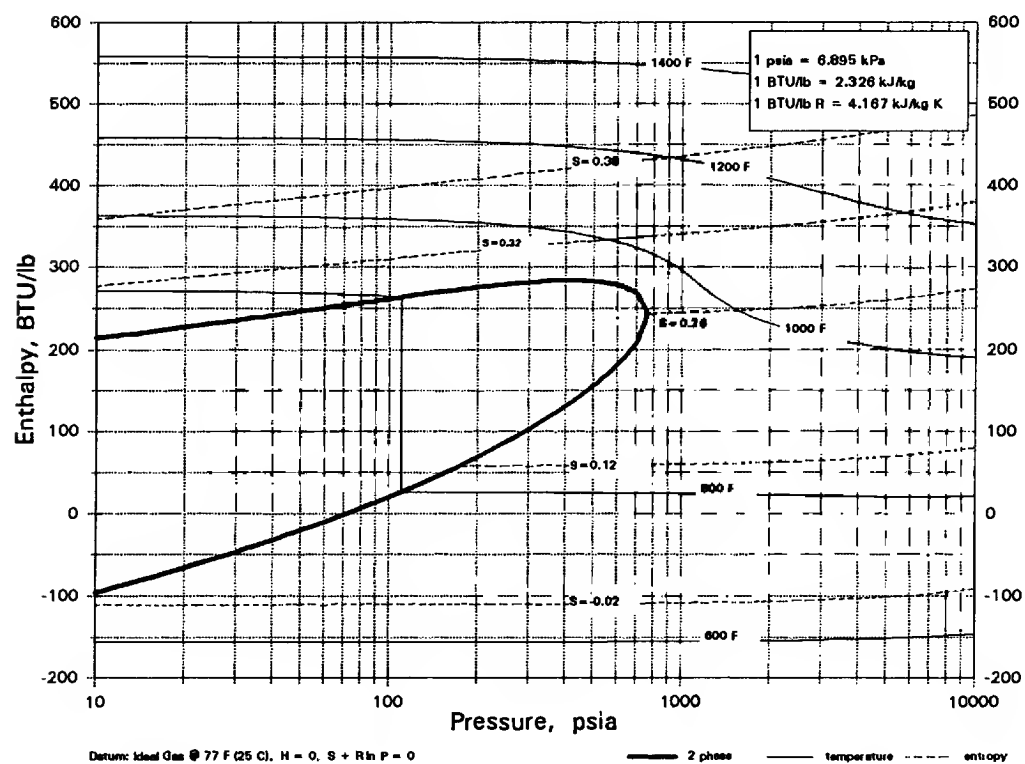
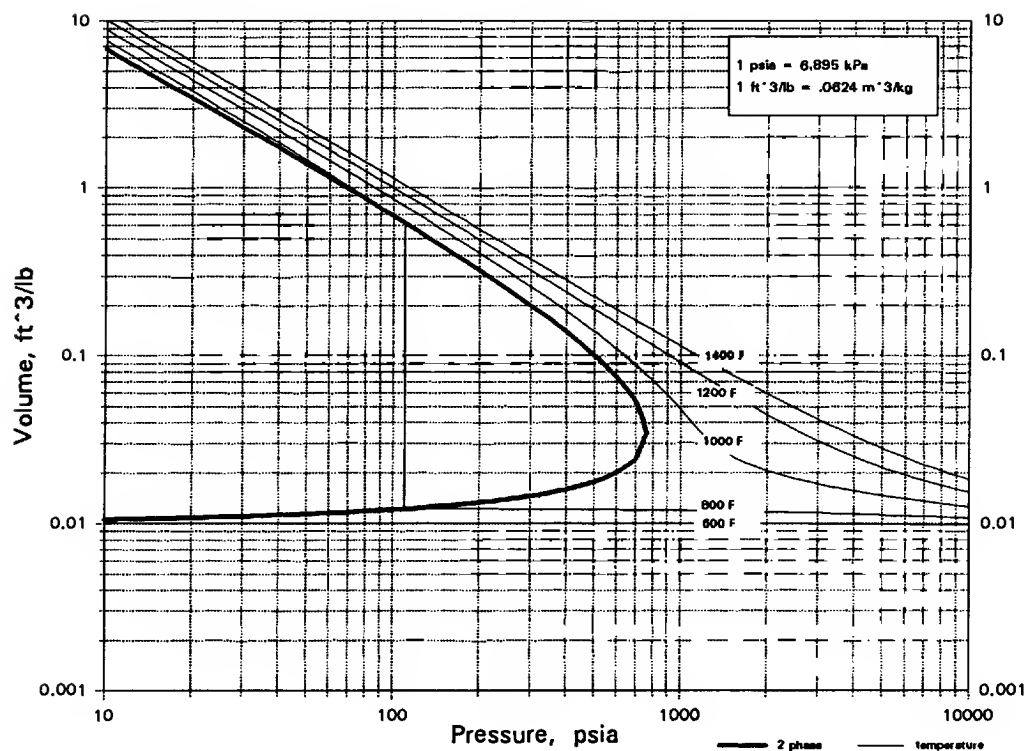
C6H8O4

DIMETHYL MALEATE



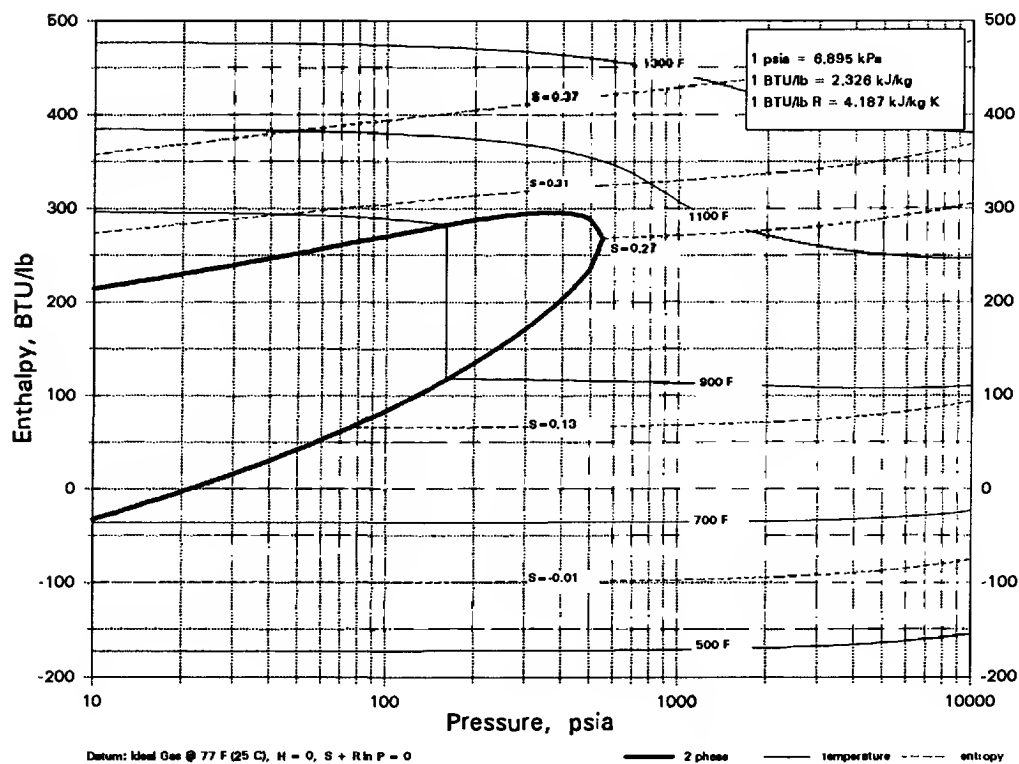
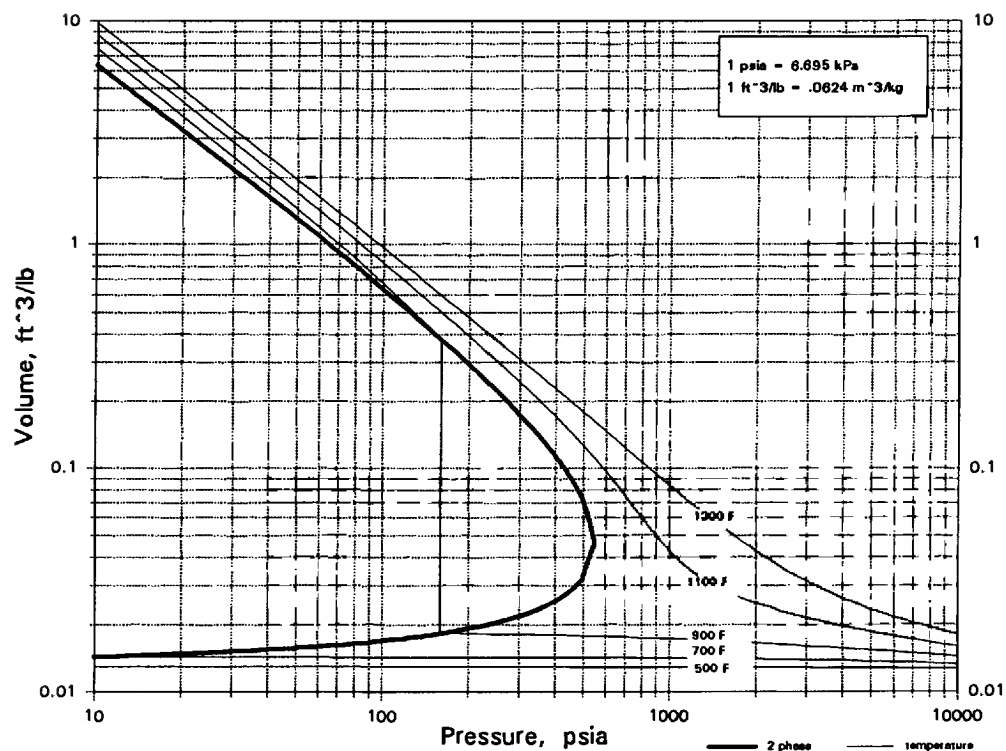
C6H8O6

ASCORBIC ACID



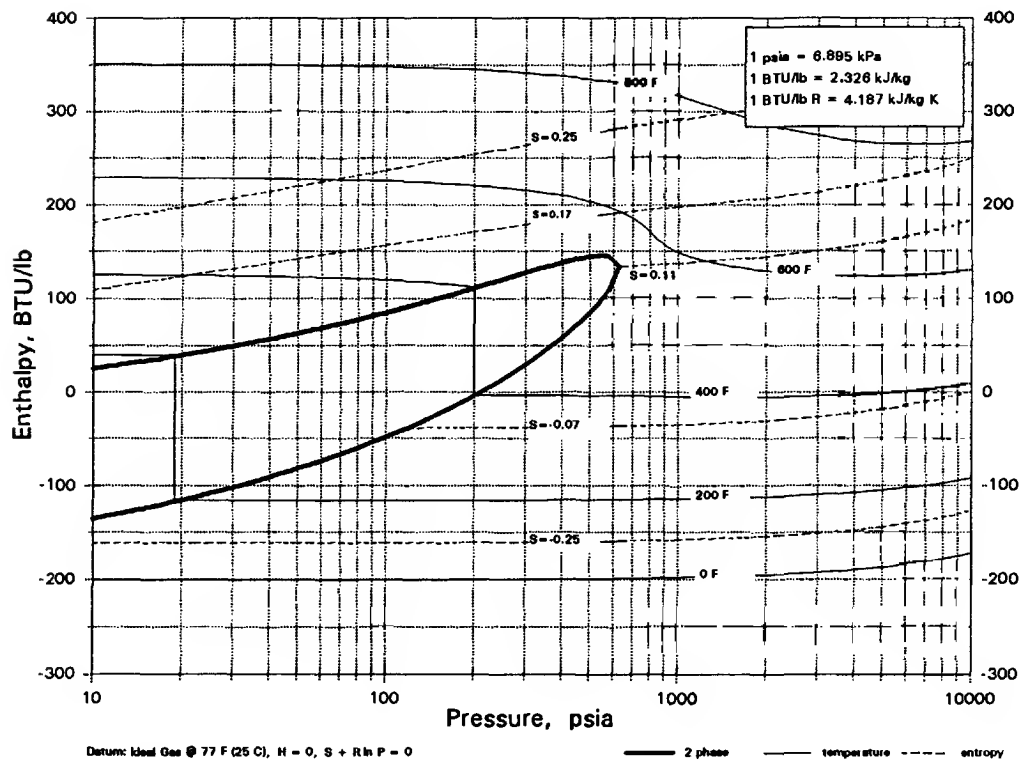
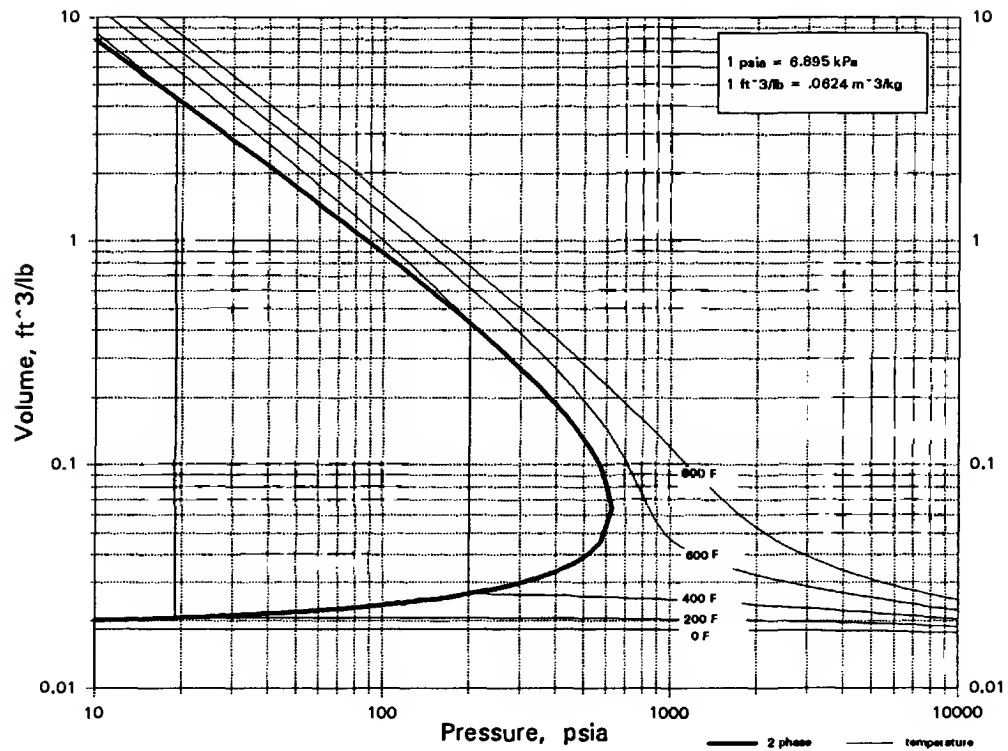
C6H8O7

CITRIC ACID



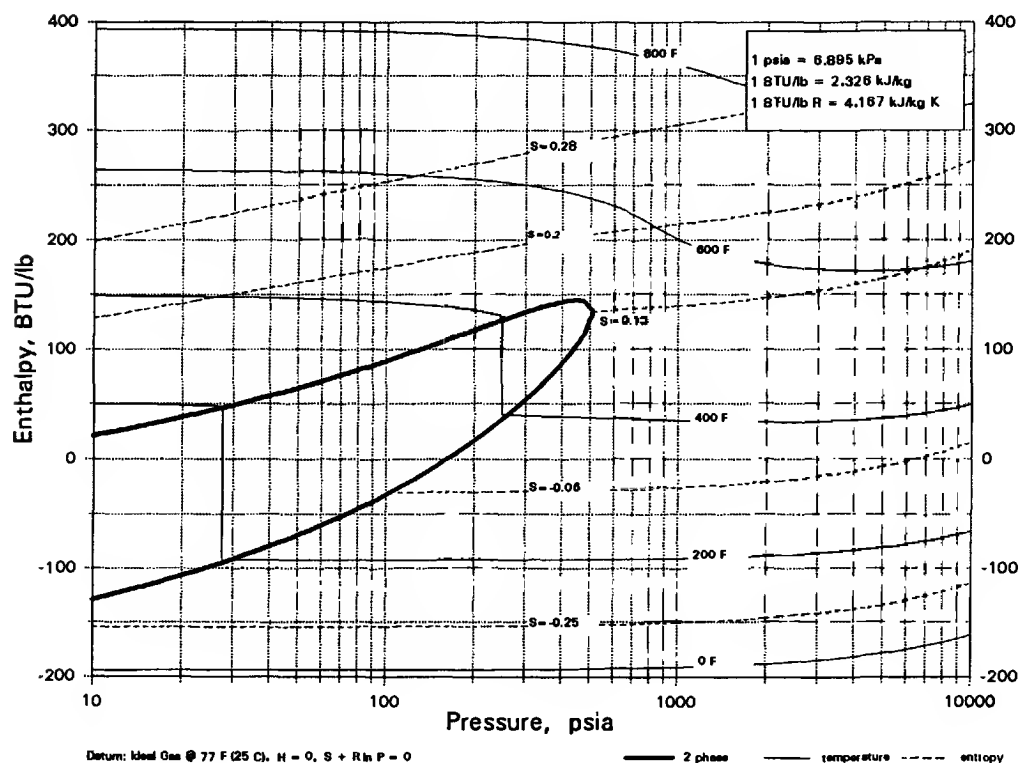
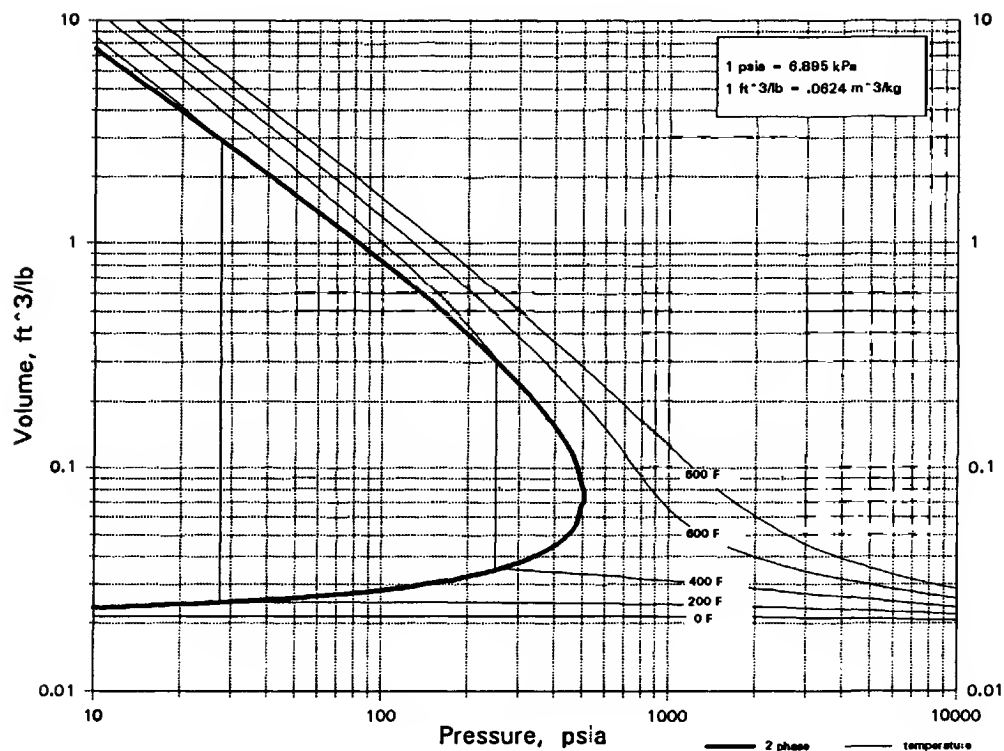
C6H10

CYCLOHEXENE



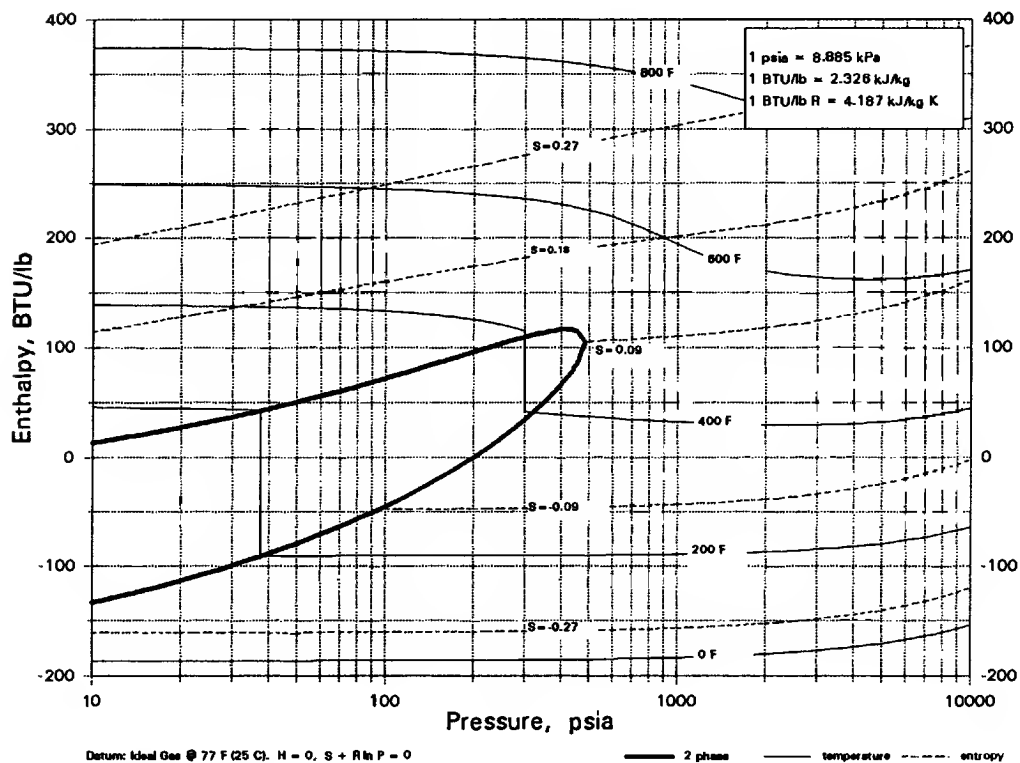
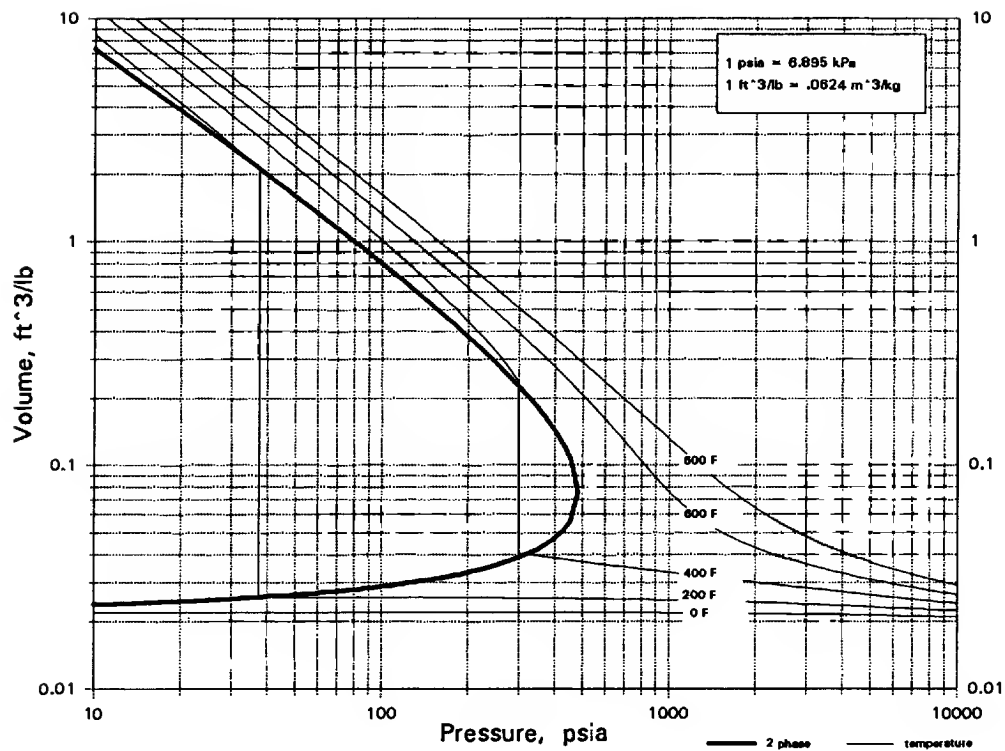
C6H10

2-3-DIMETHYL-1-3-BUTADIENE



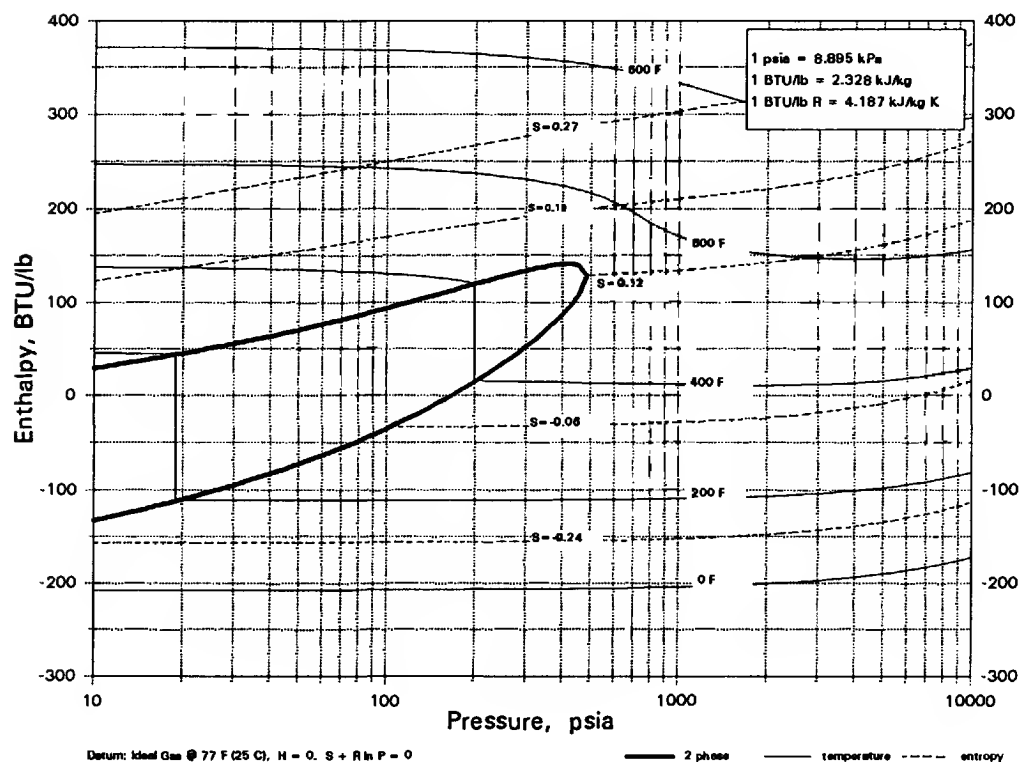
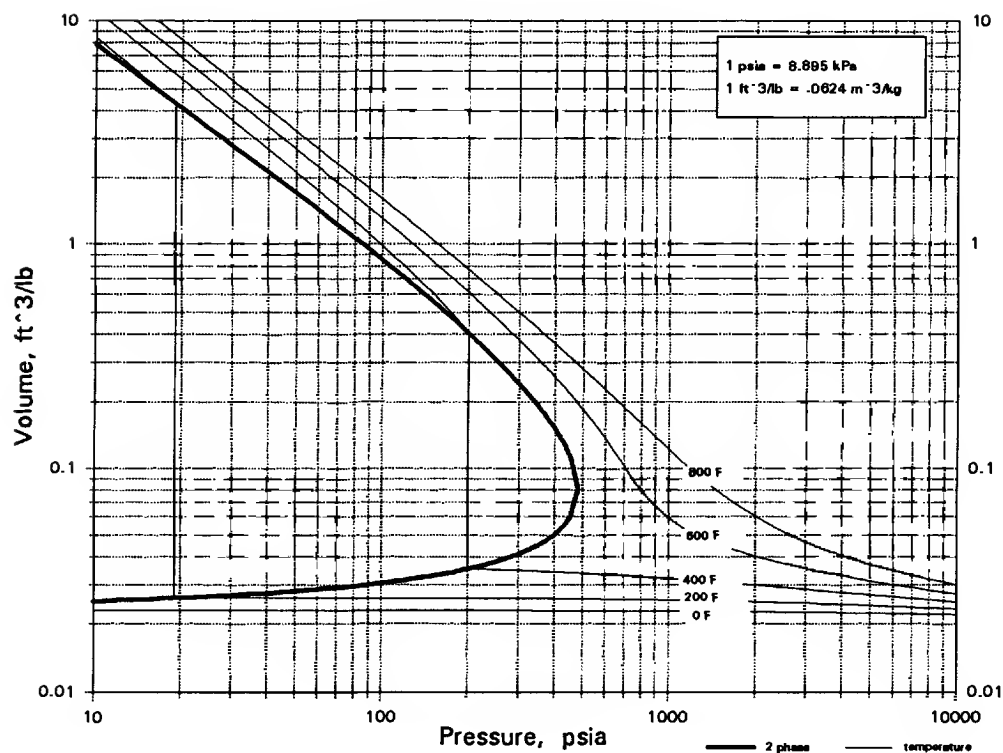
C6H10

1-5-HEXADIENE



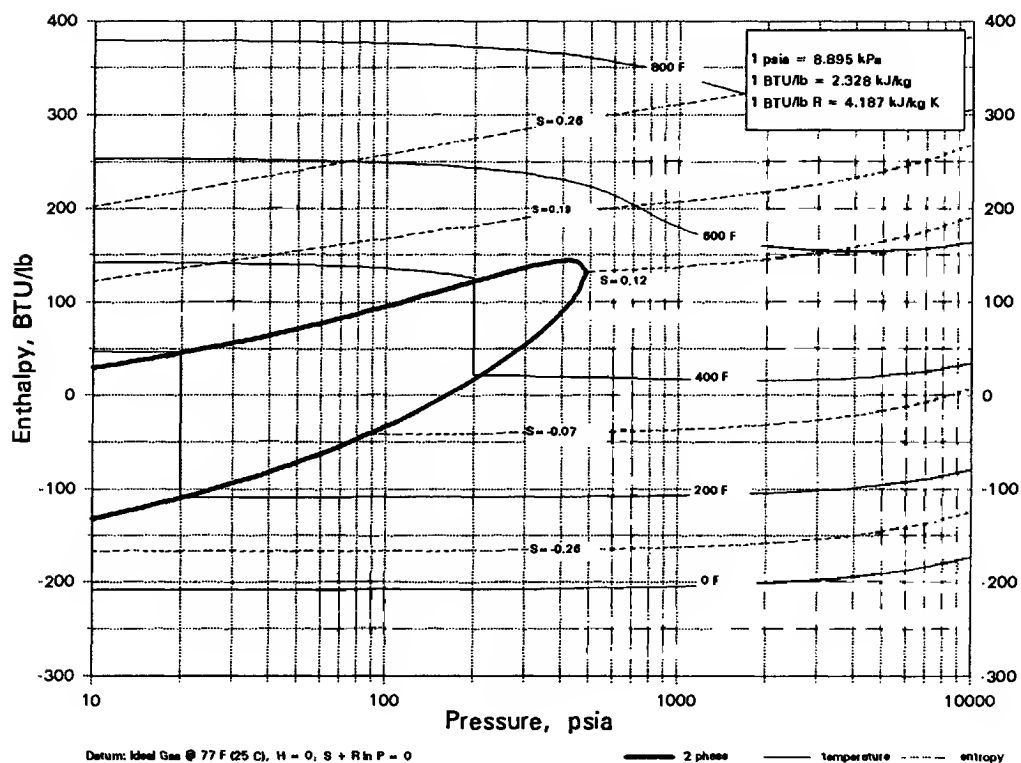
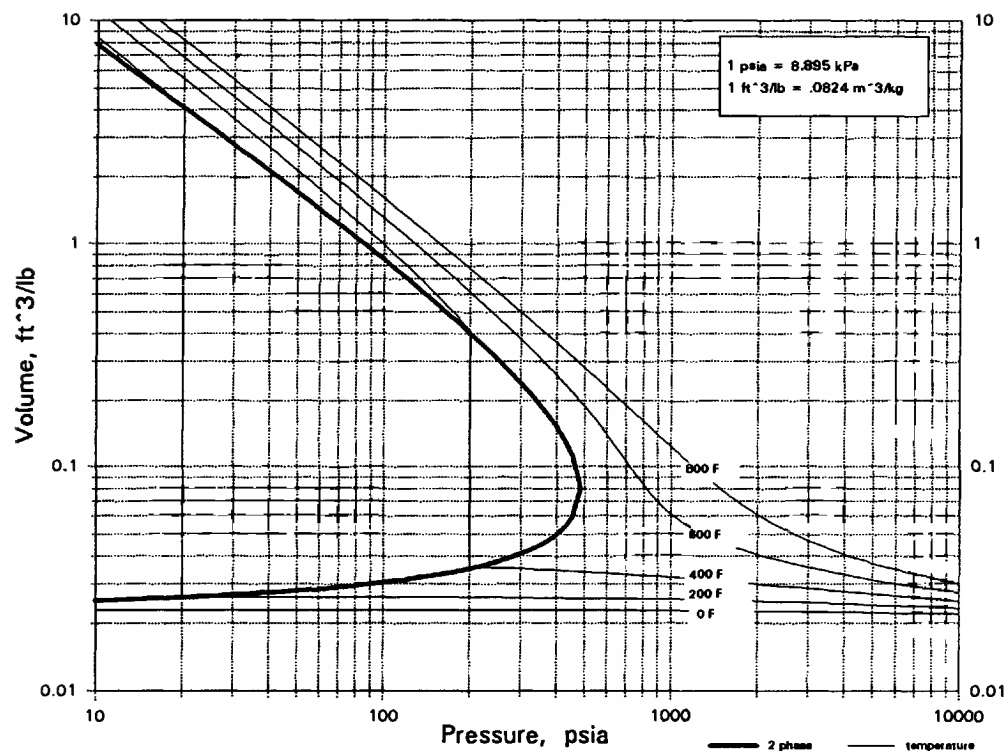
C6H10

cis-trans-2-4-HEXADIENE



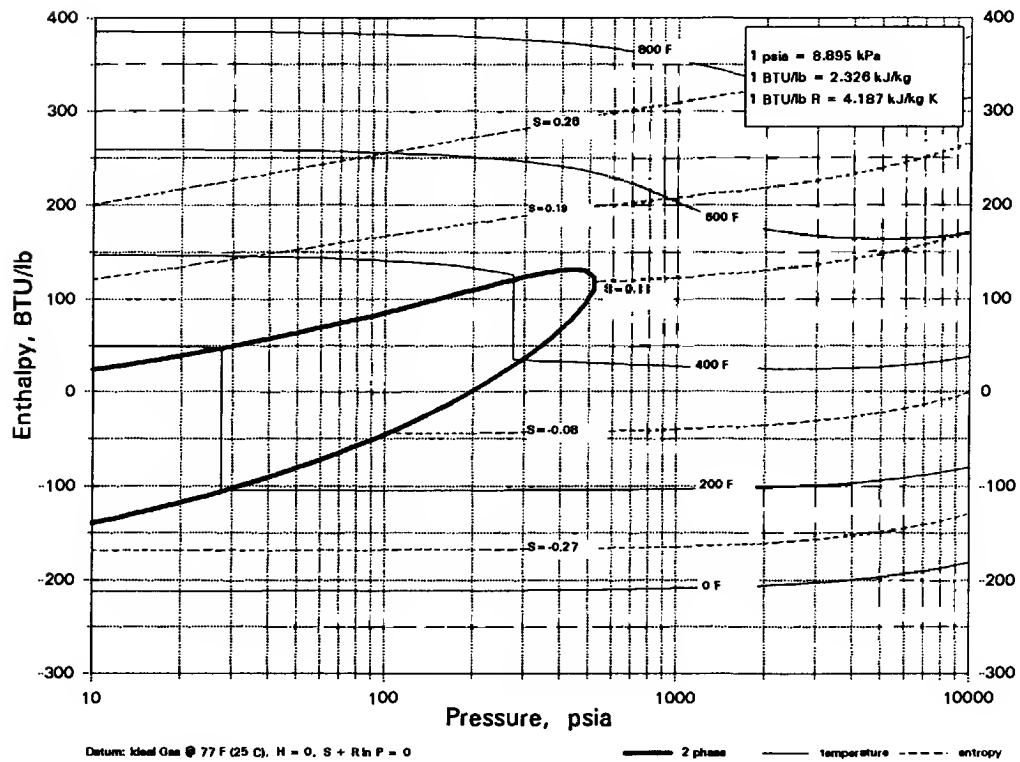
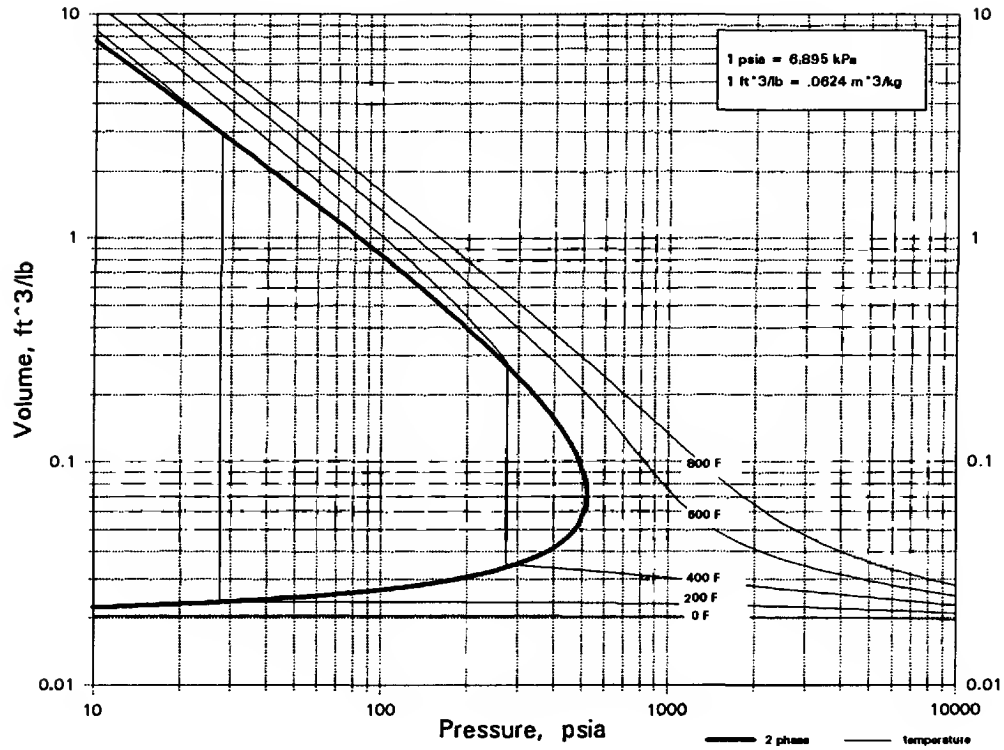
C6H10

trans-trans-2,4-HEXADIENE



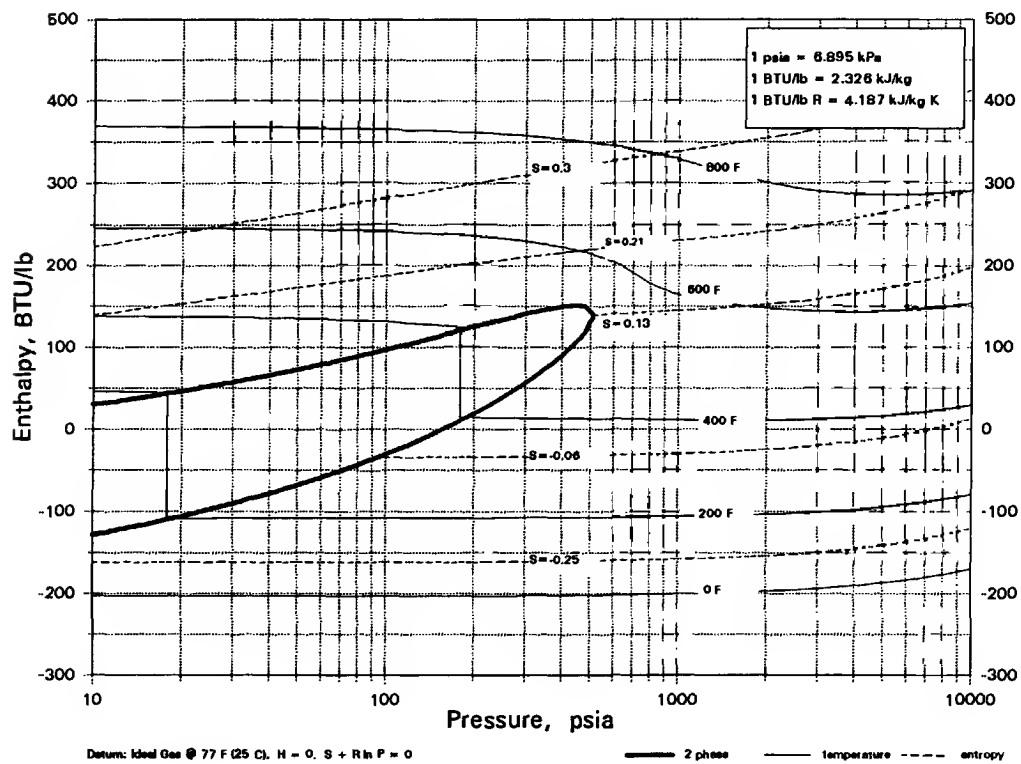
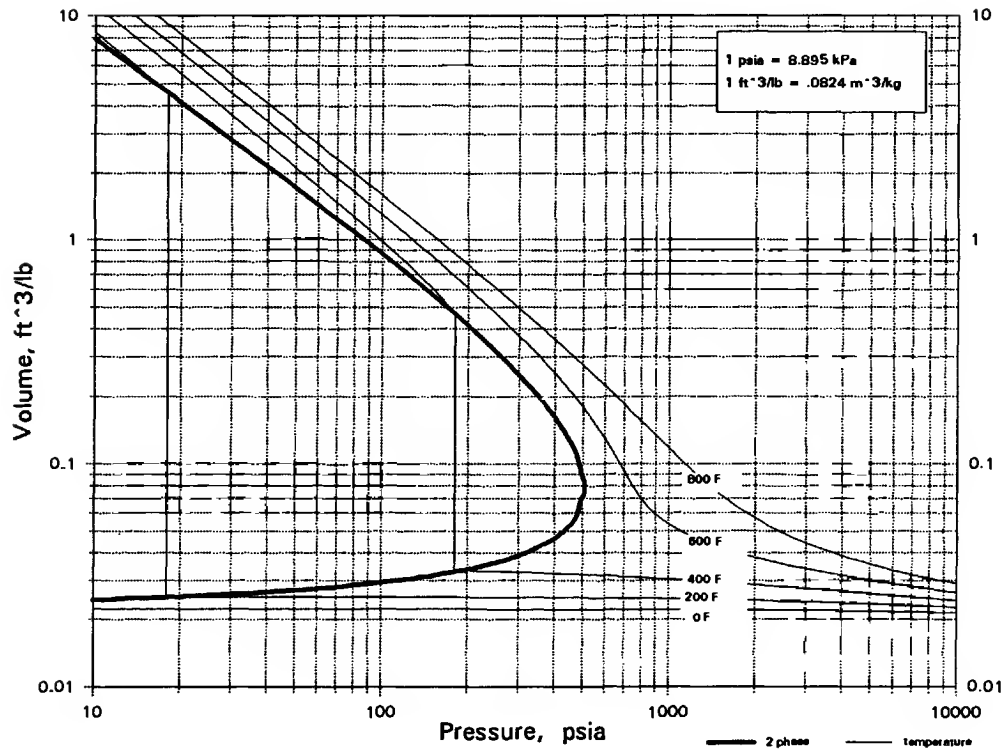
C6H10

1-HEXYNE



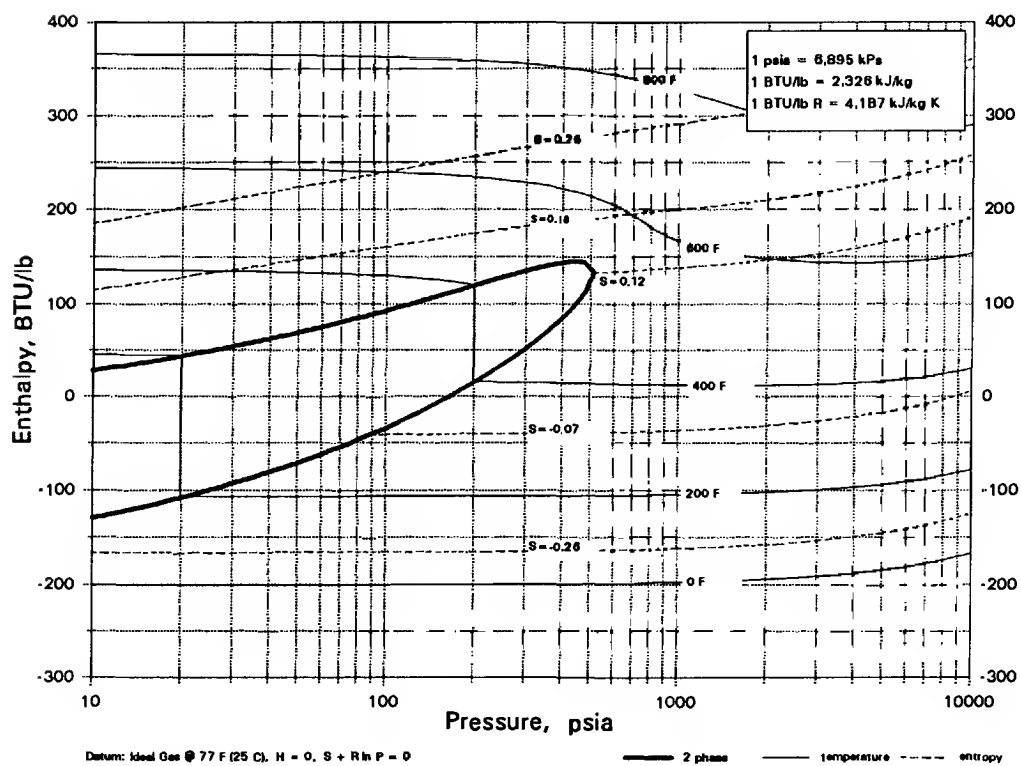
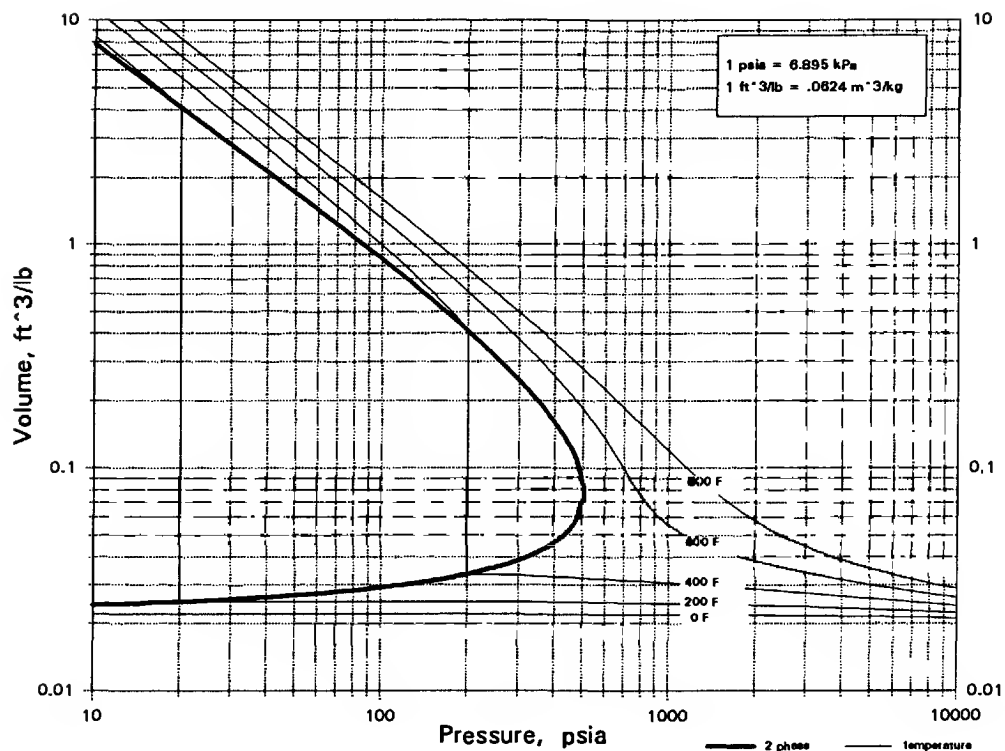
C6H10

2-HEXYNE



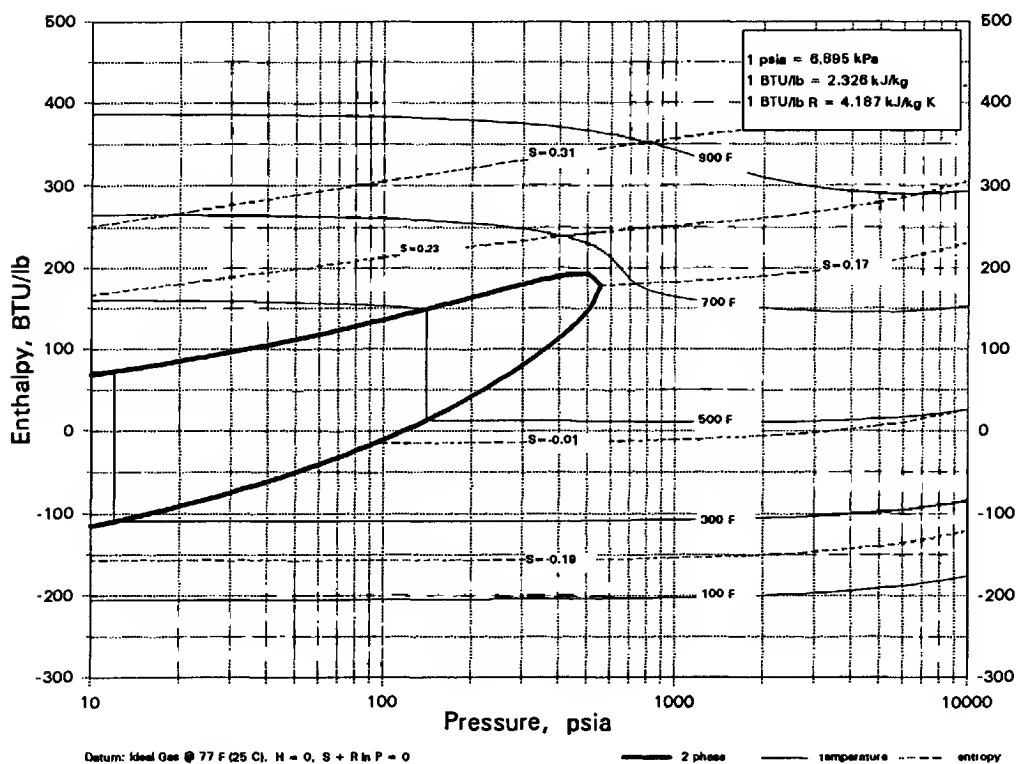
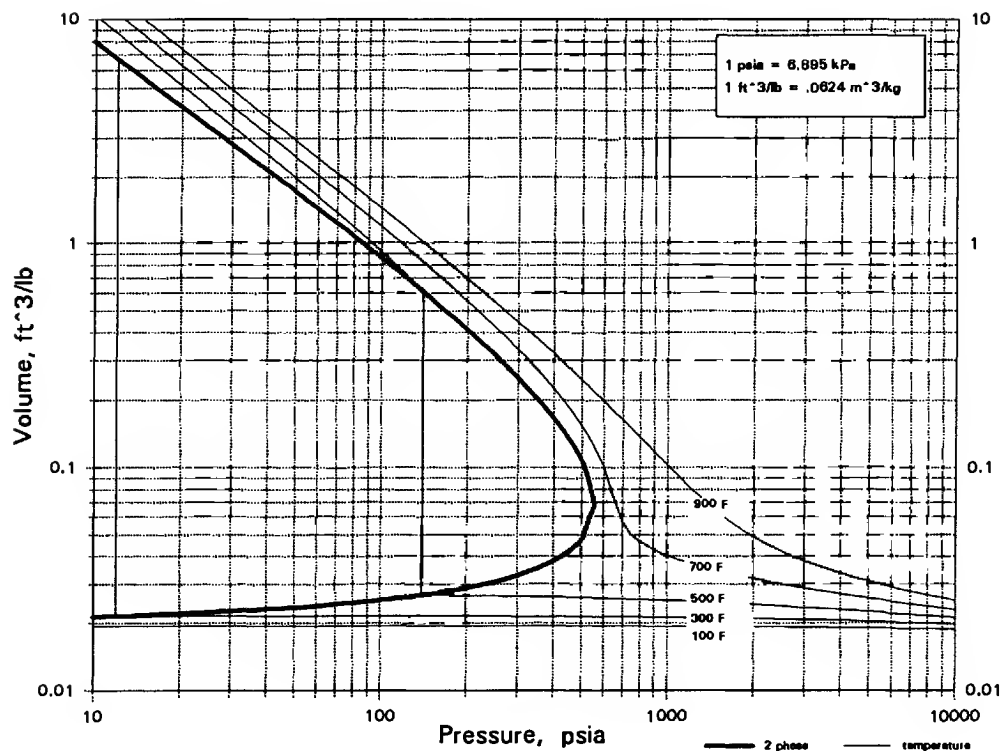
C6H10

3-HEXYNE



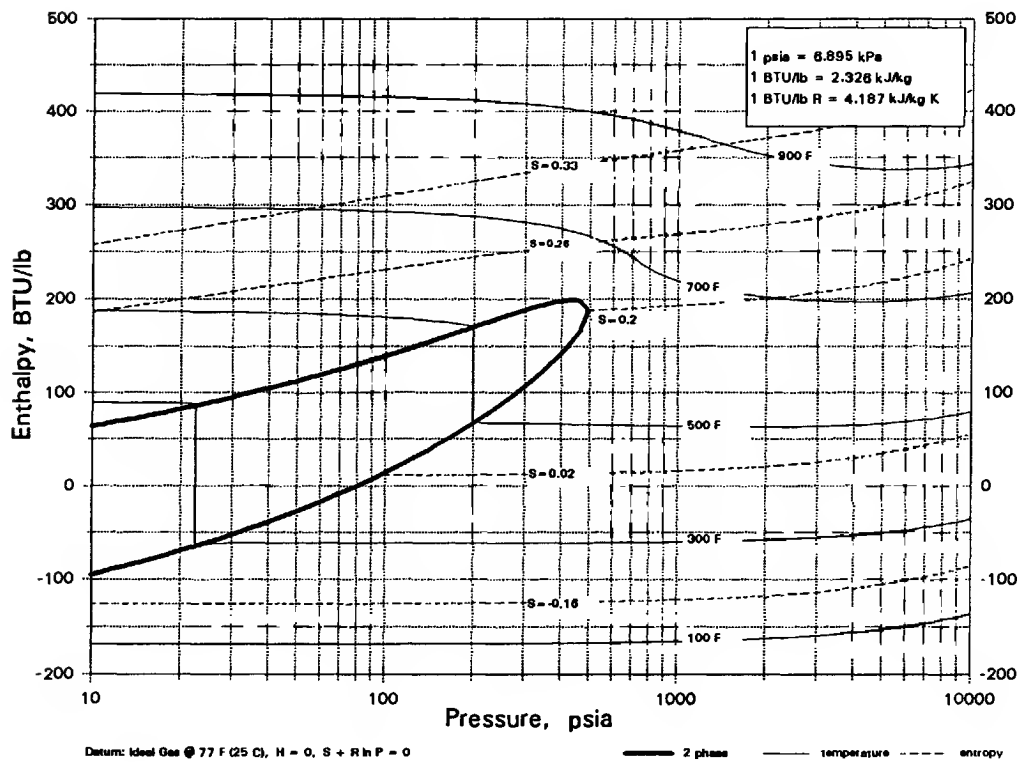
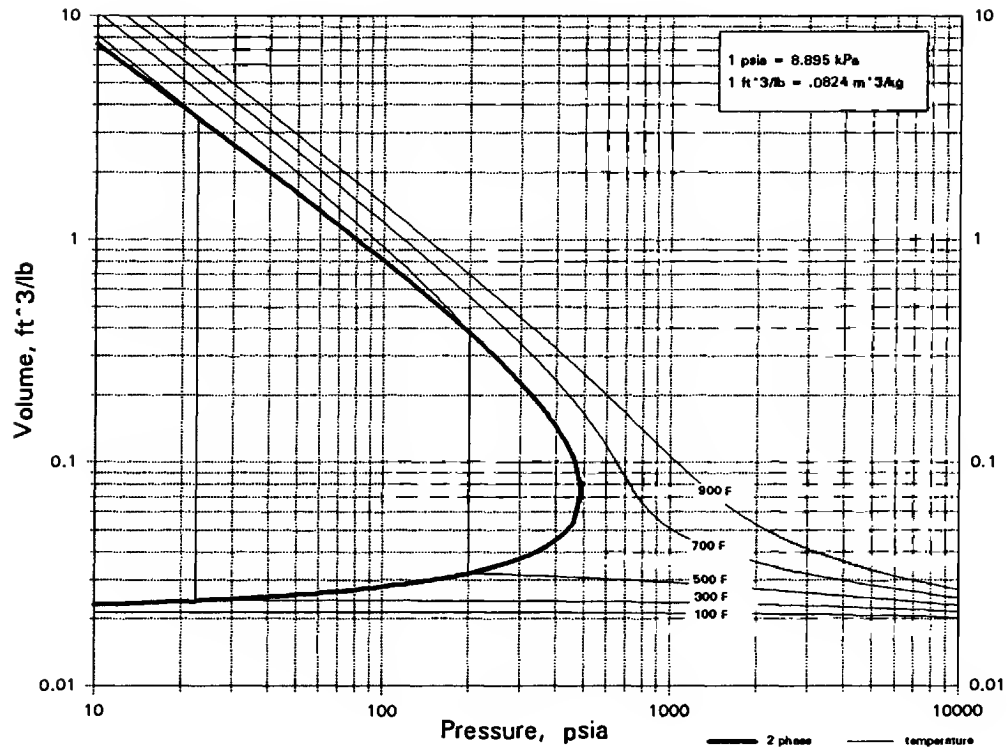
C6H10O

CYCLOHEXANONE



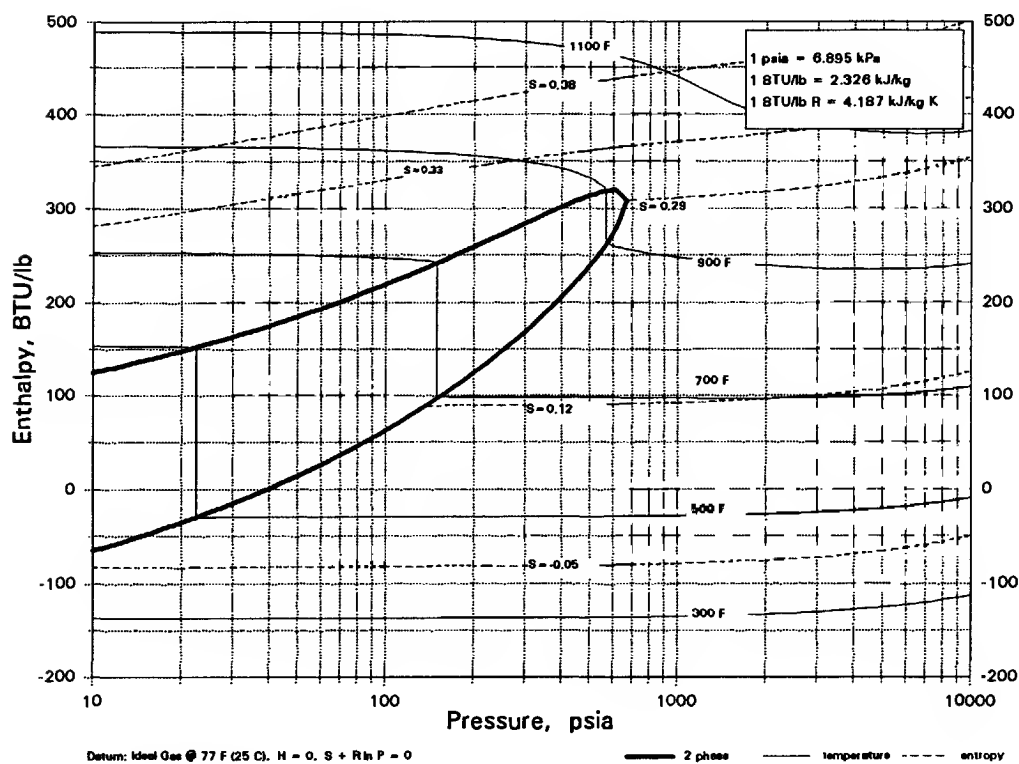
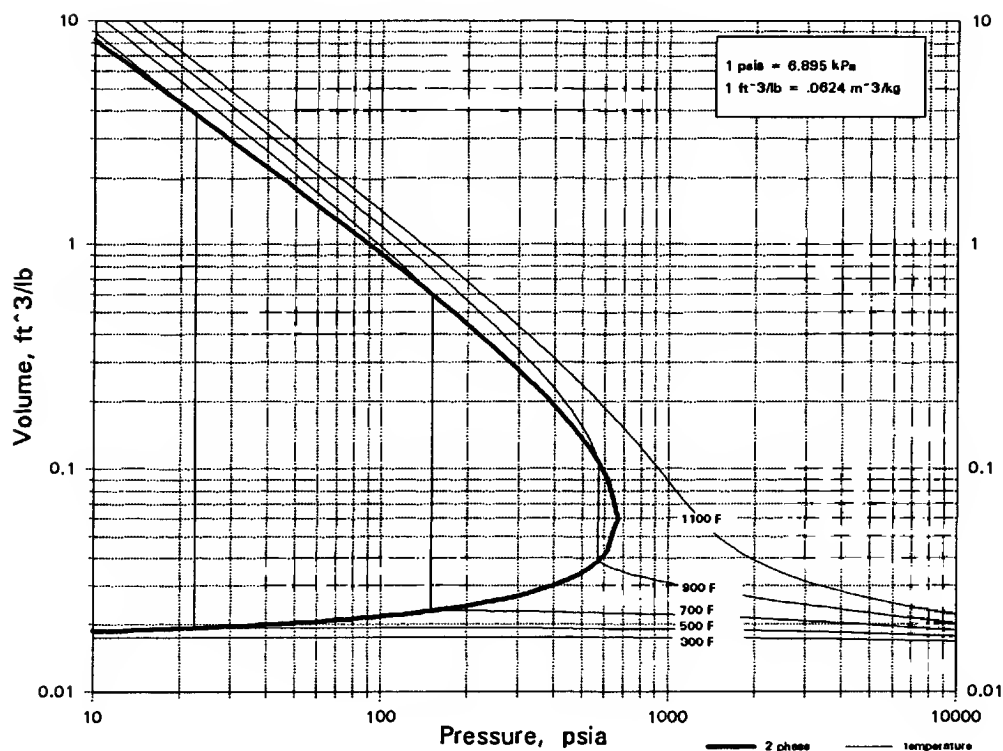
C6H10O

MESITYL OXIDE



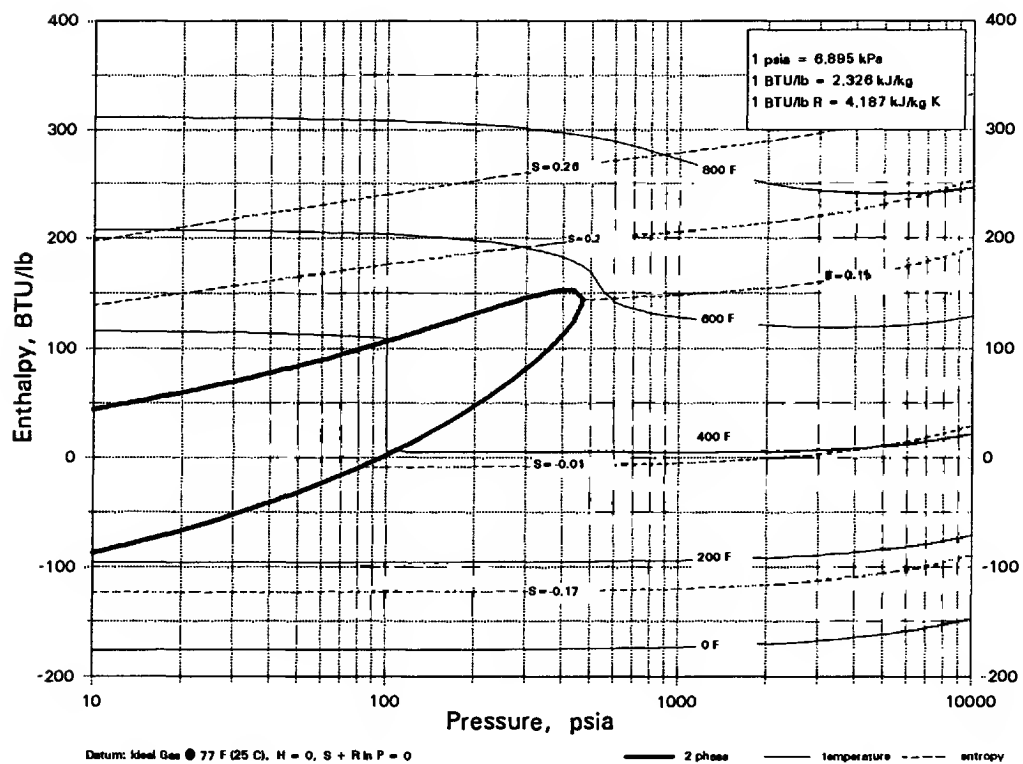
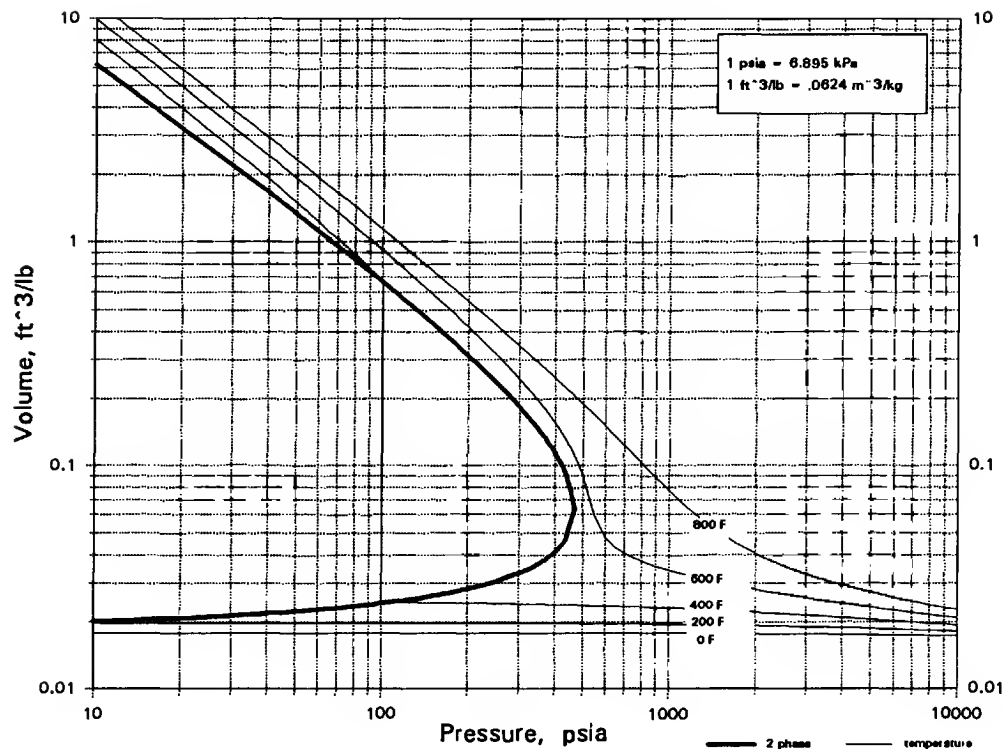
C6H10O2

epsilon-CAPROLACTONE



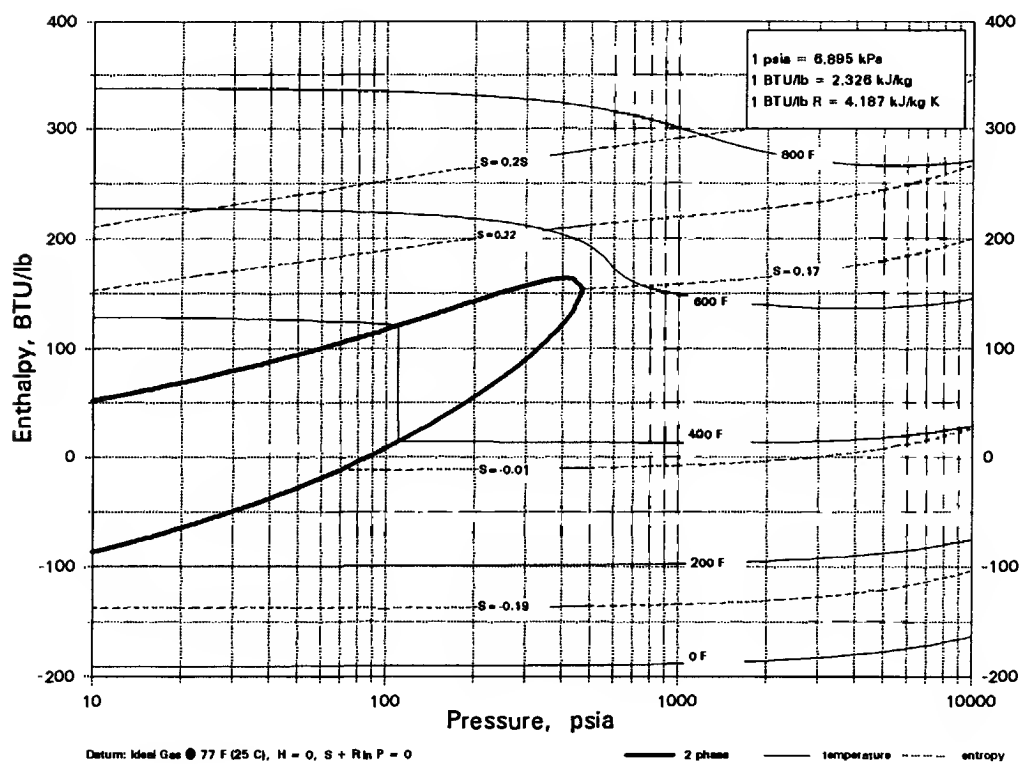
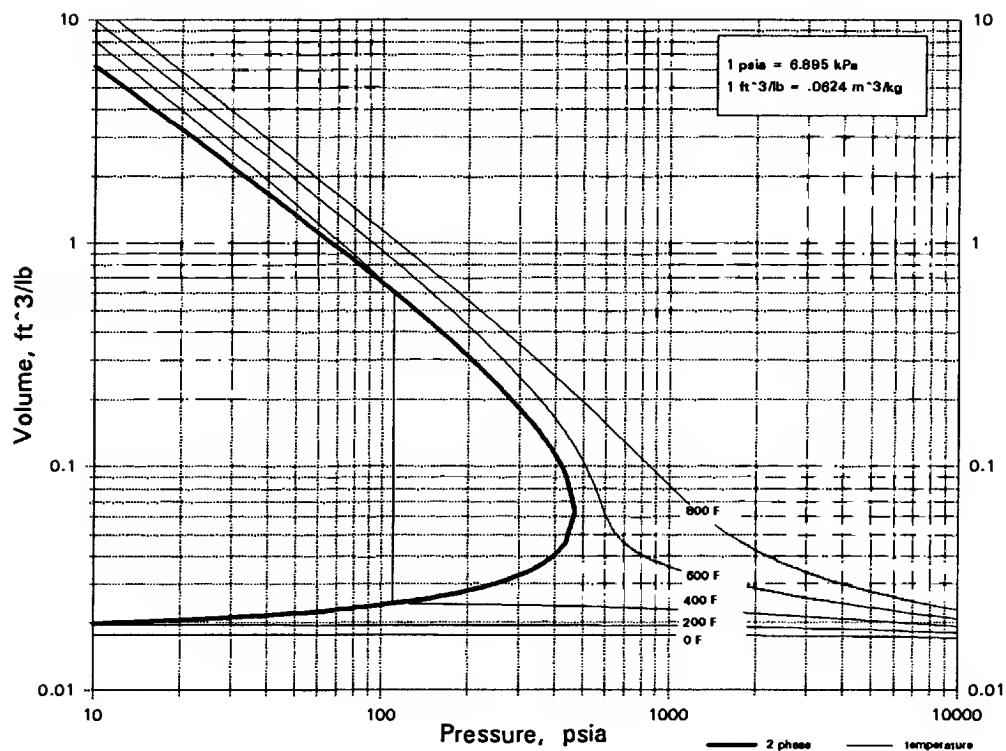
C6H10O2

ETHYL METHACRYLATE



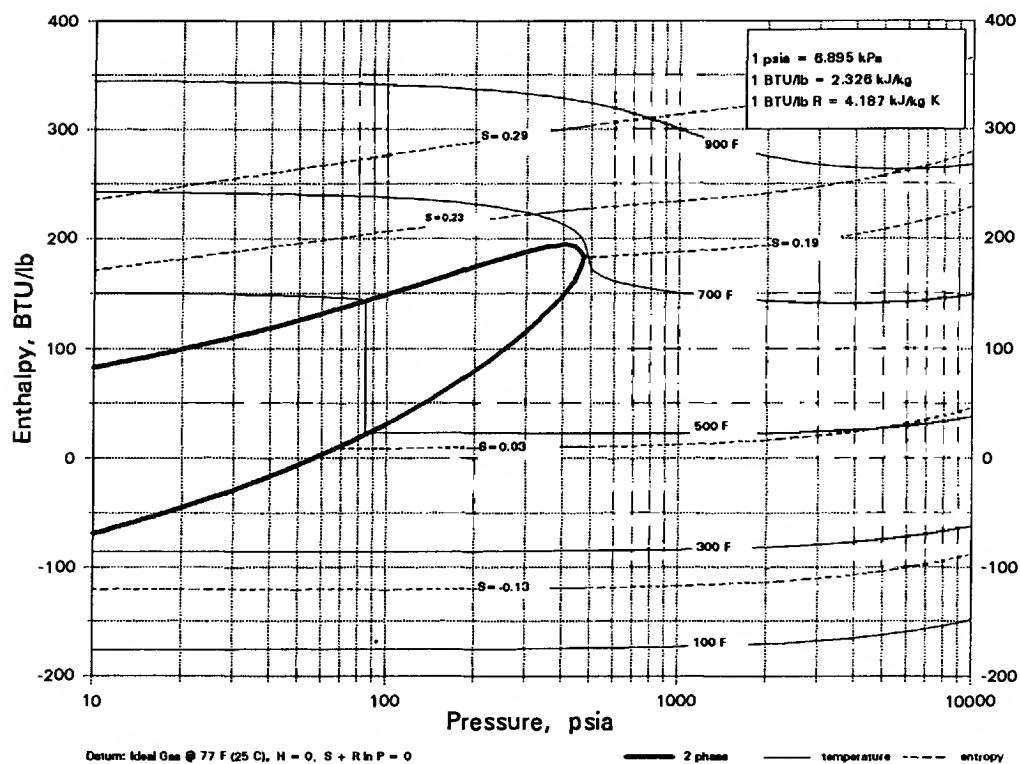
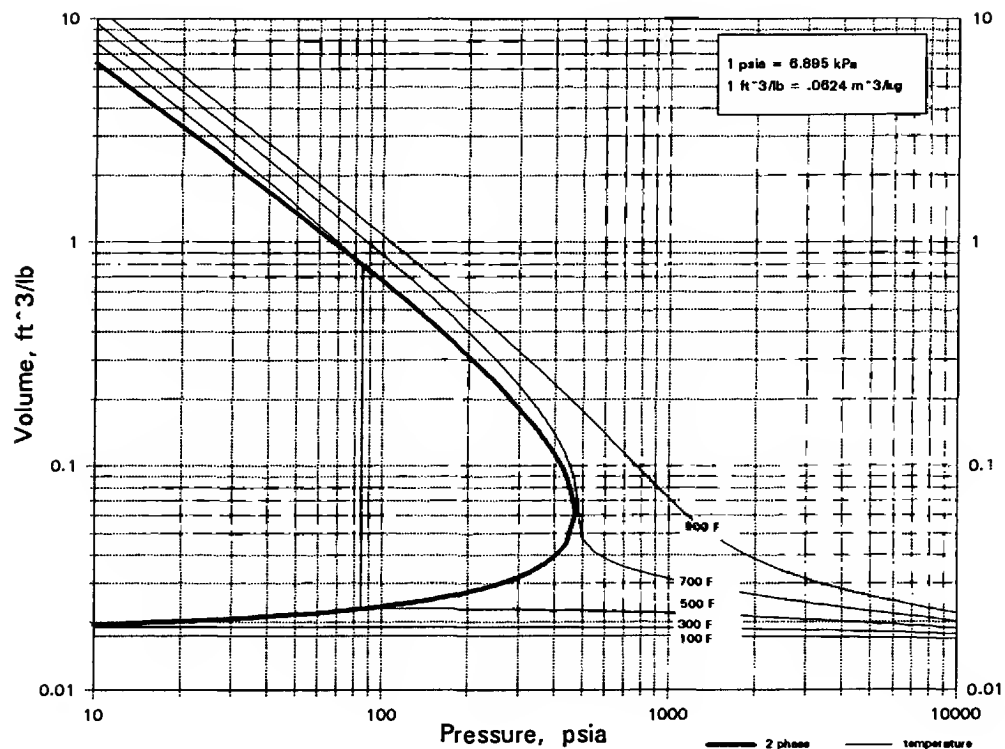
C6H10O2

n-PROPYL ACRYLATE



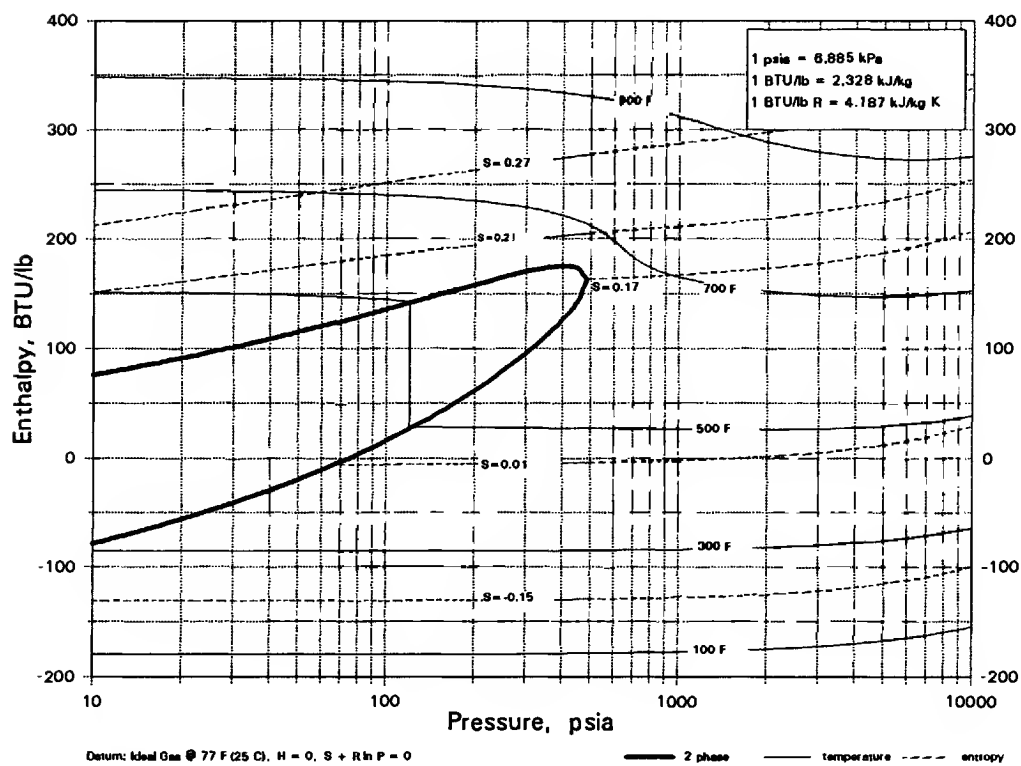
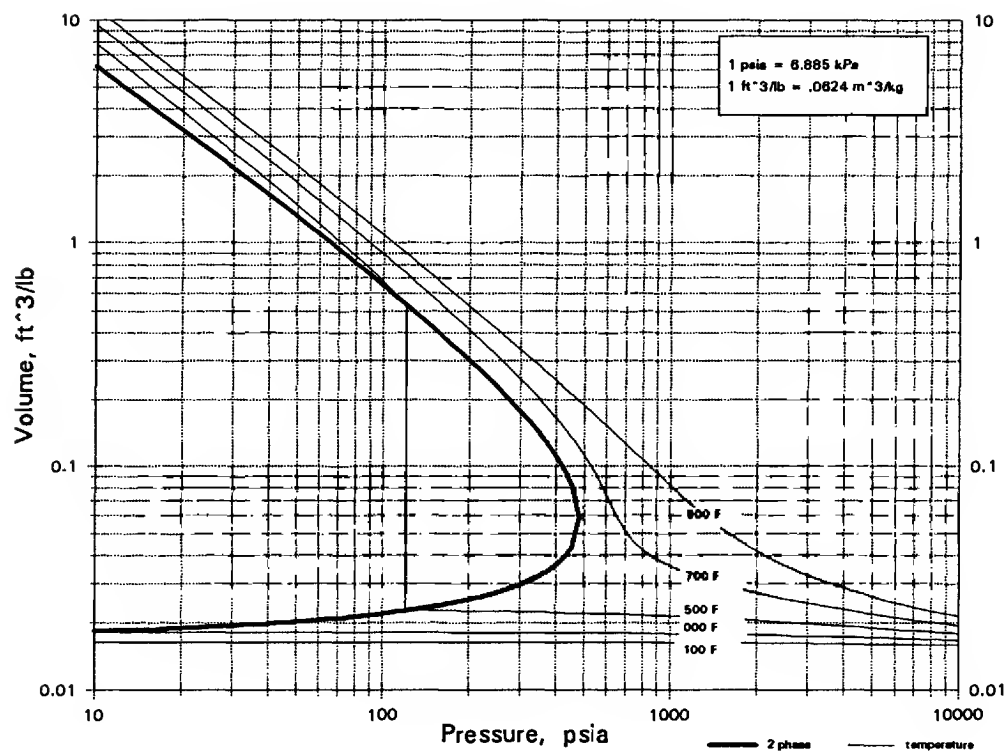
C6H10O3

ETHYLACETOACETATE



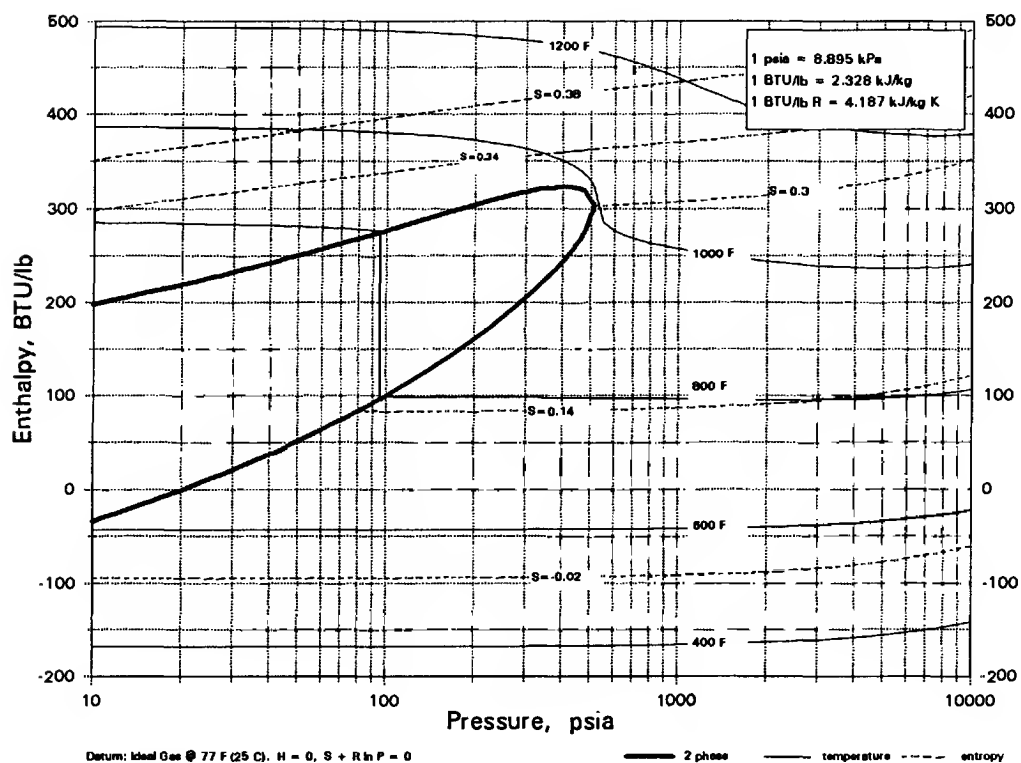
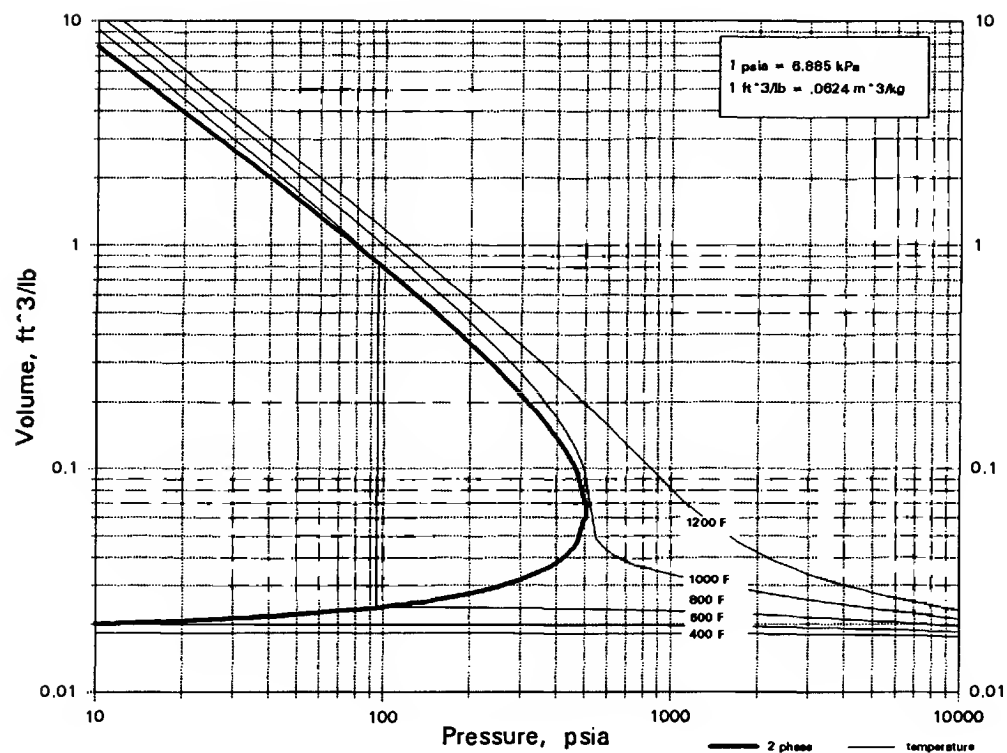
C6H10O3

PROPIONIC ANHYDRIDE



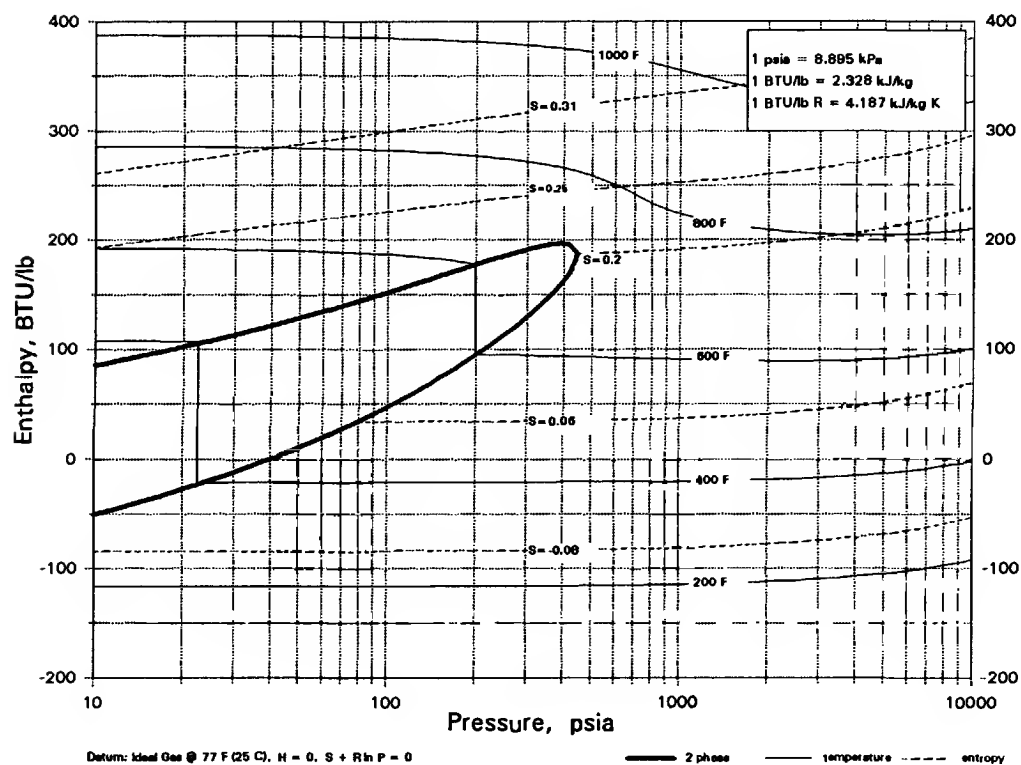
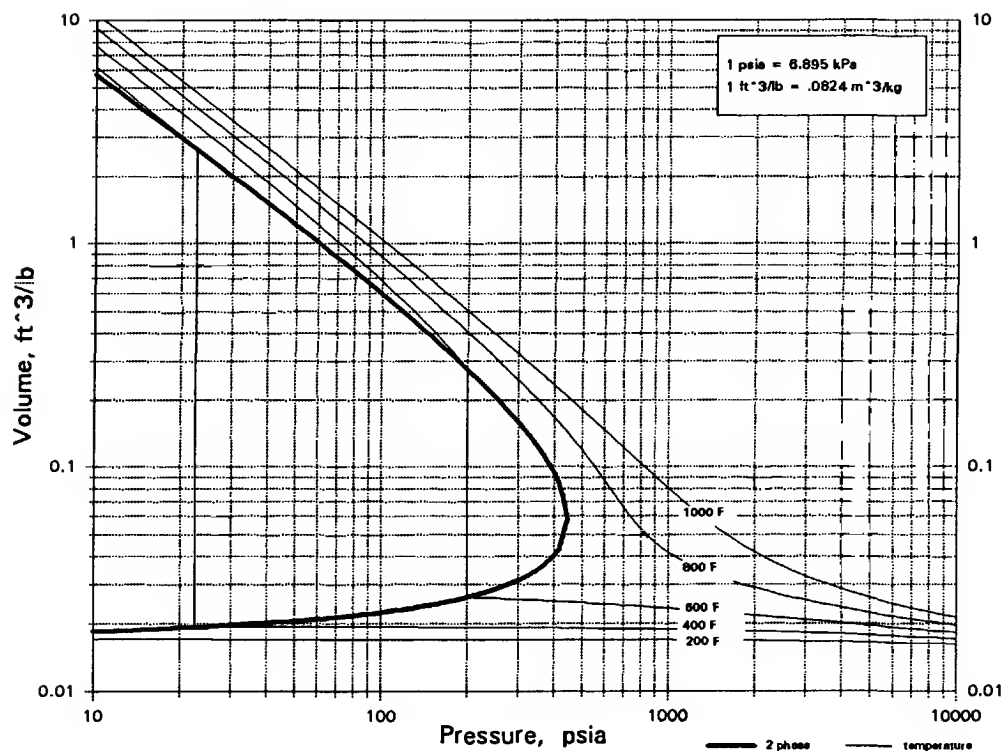
C6H10O4

ADIPIC ACID



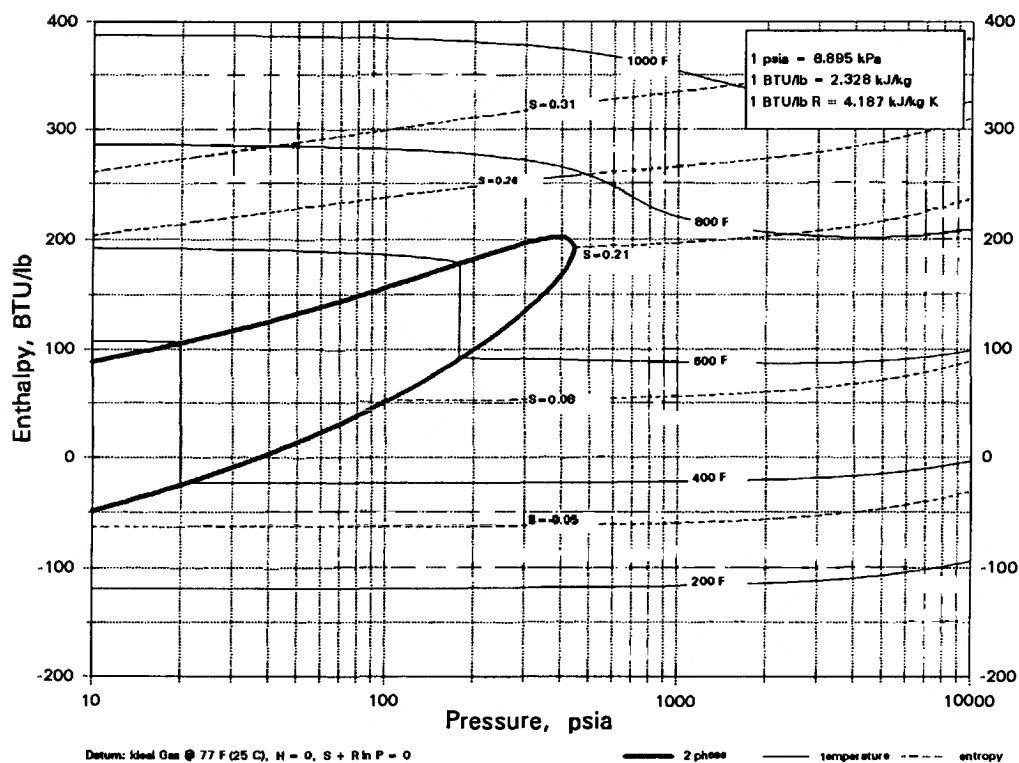
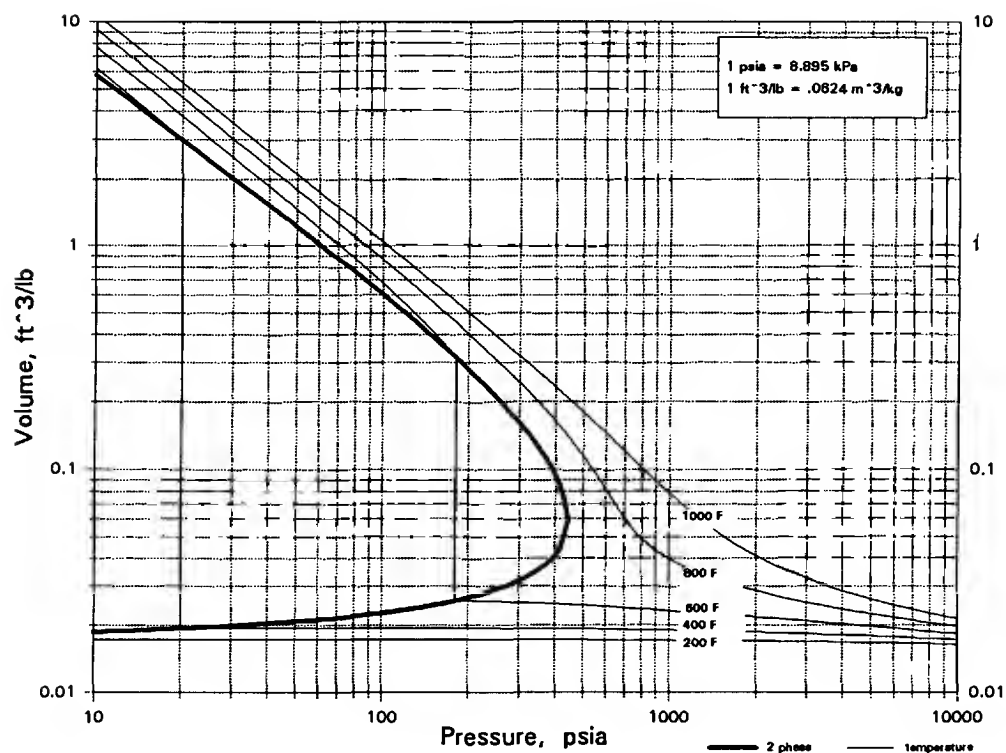
C6H10O4

DIETHYL OXALATE



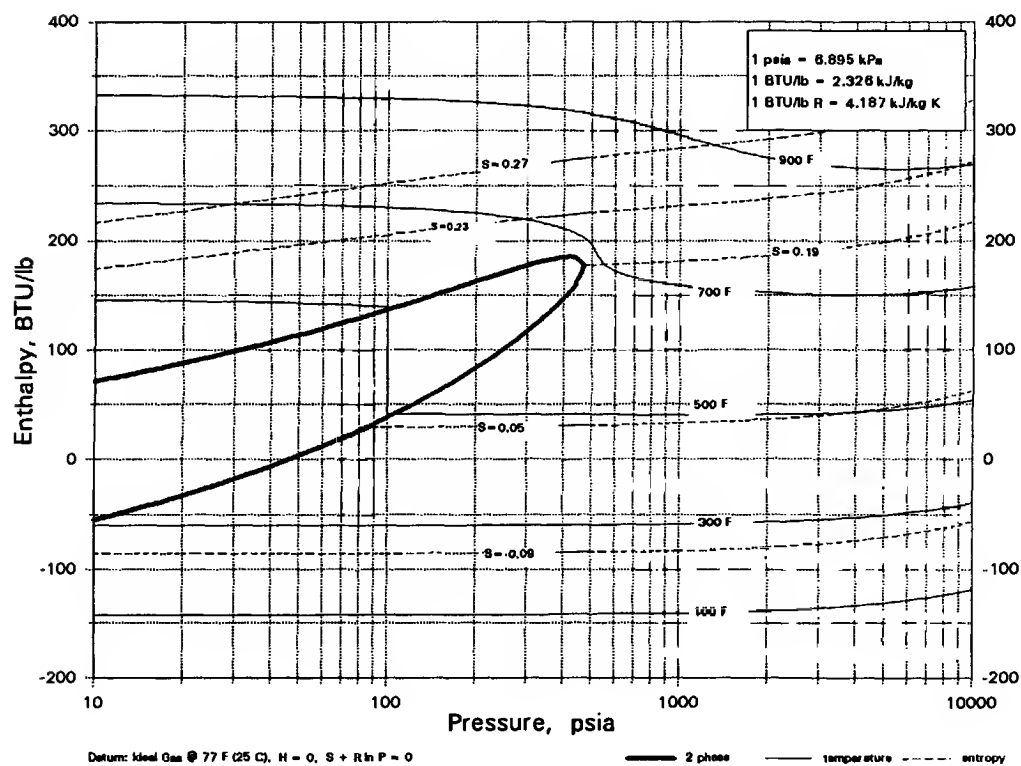
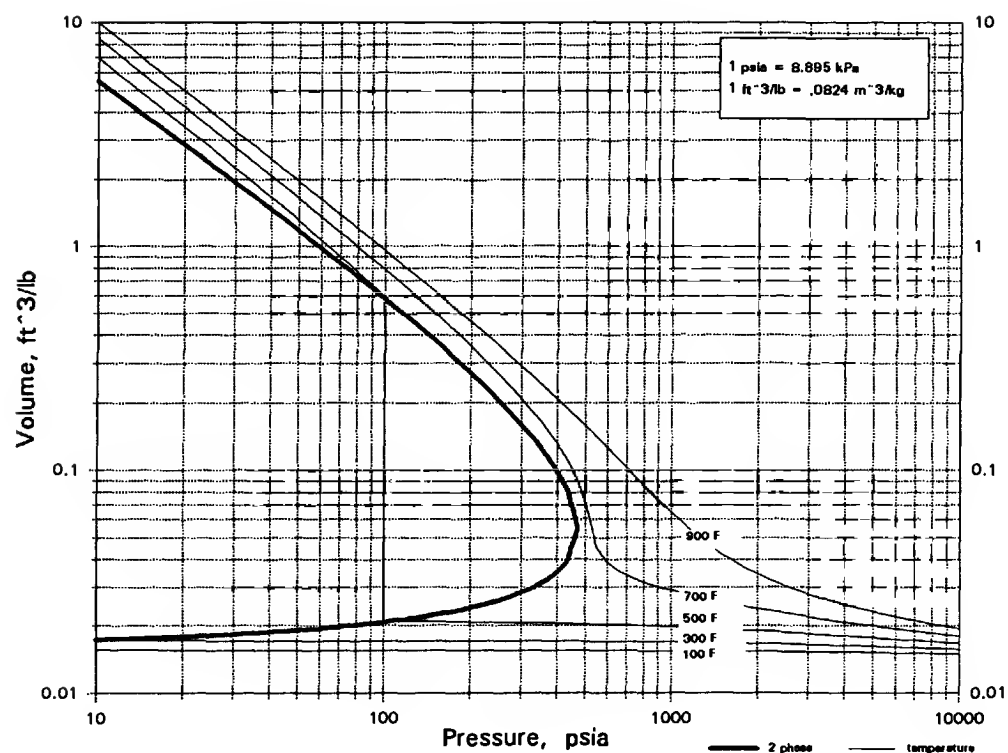
C6H10O4

ETHYLENE GLYCOL DIACETATE



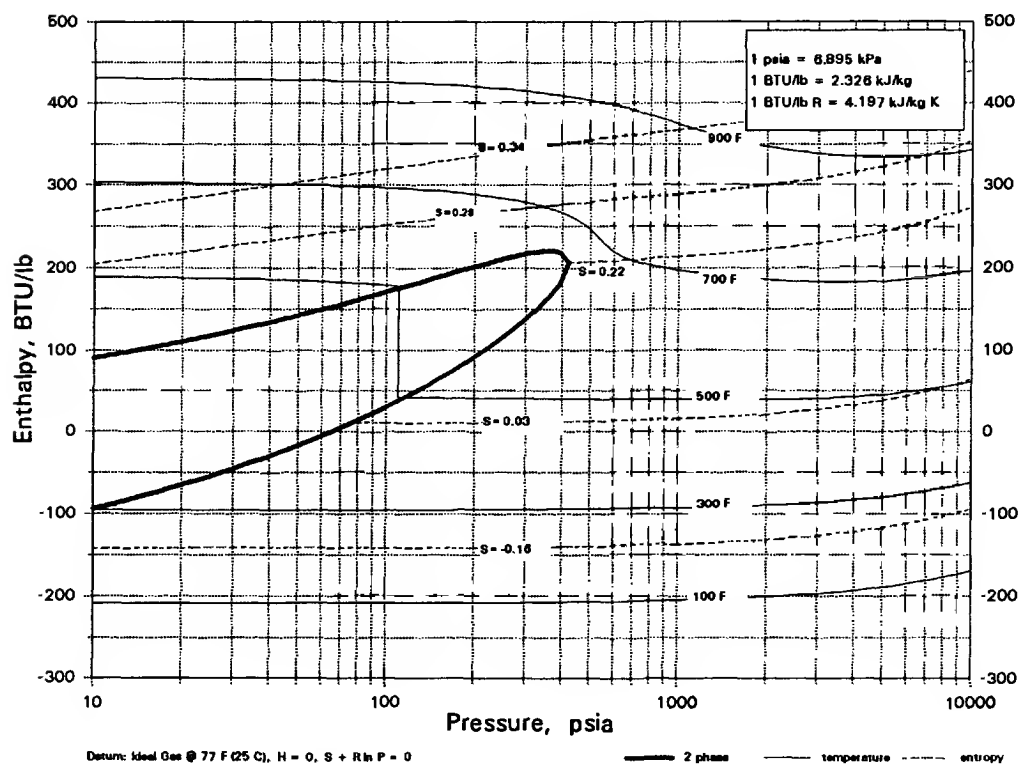
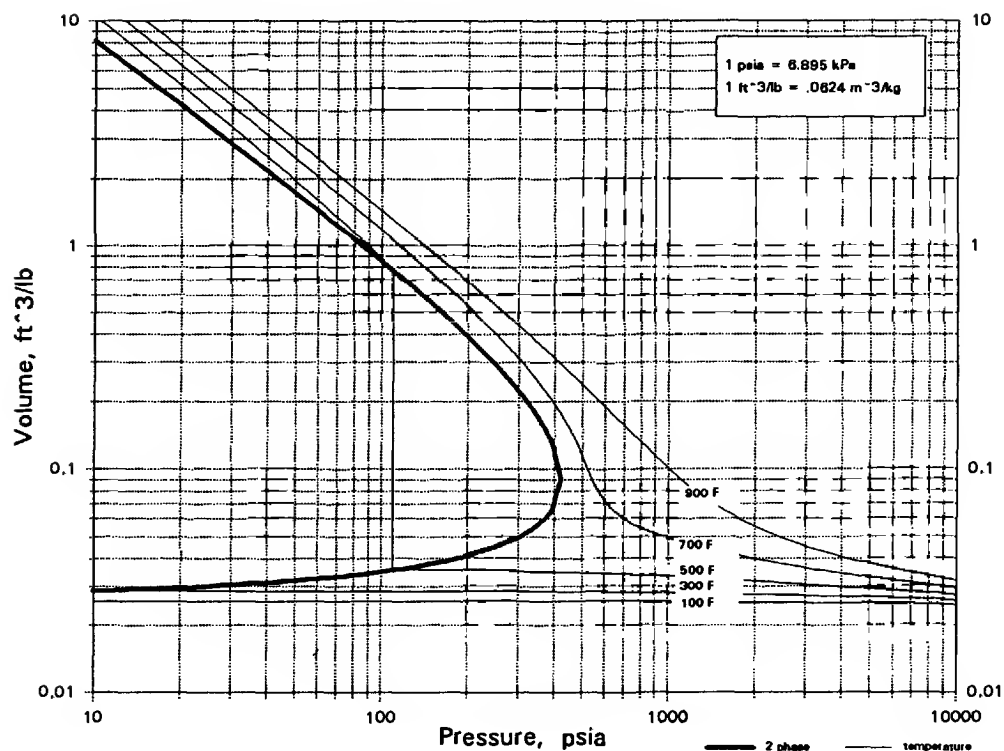
C6H10O4

ETHYLIDENE DIACETATE

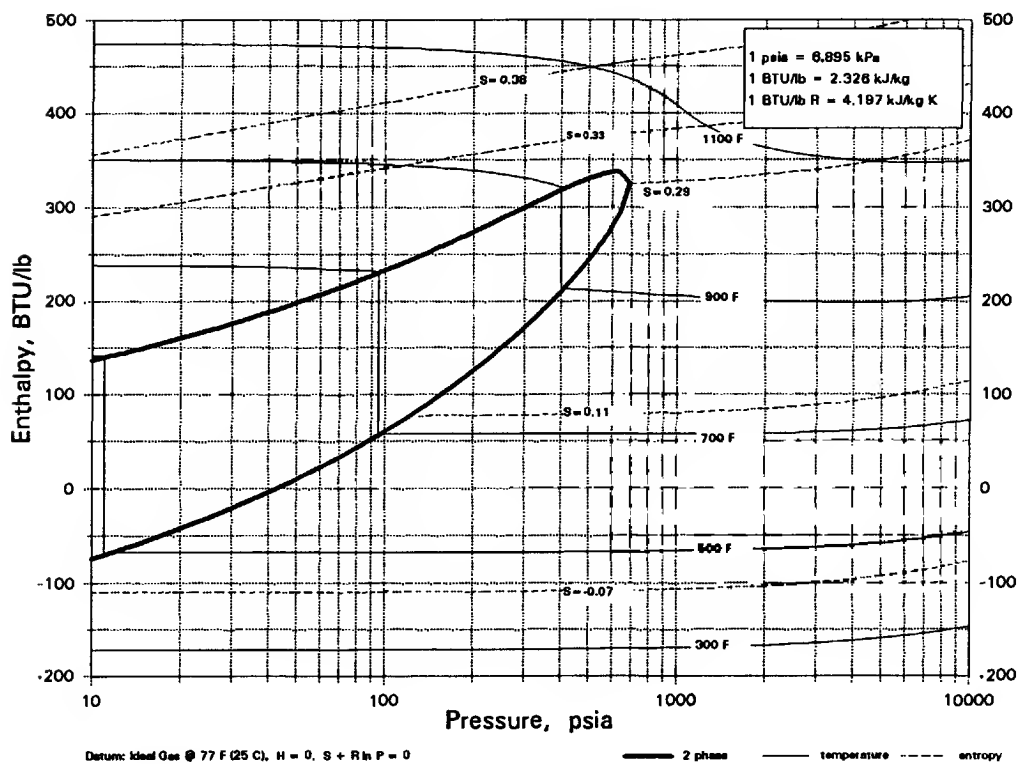
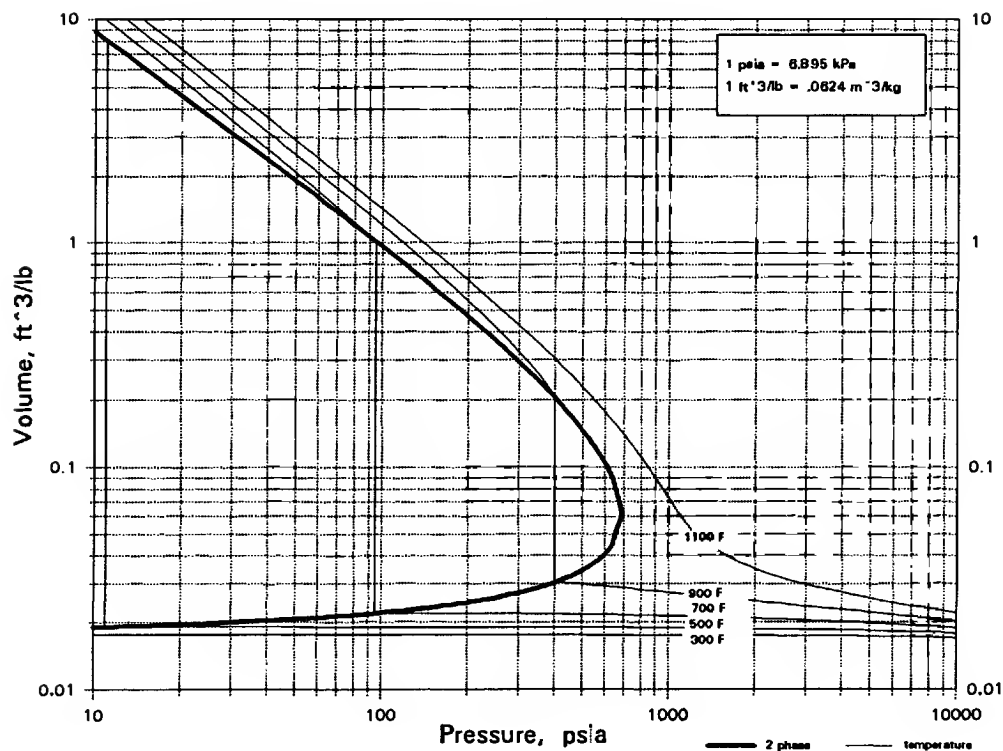


C6H11N

HEXANENITRILE

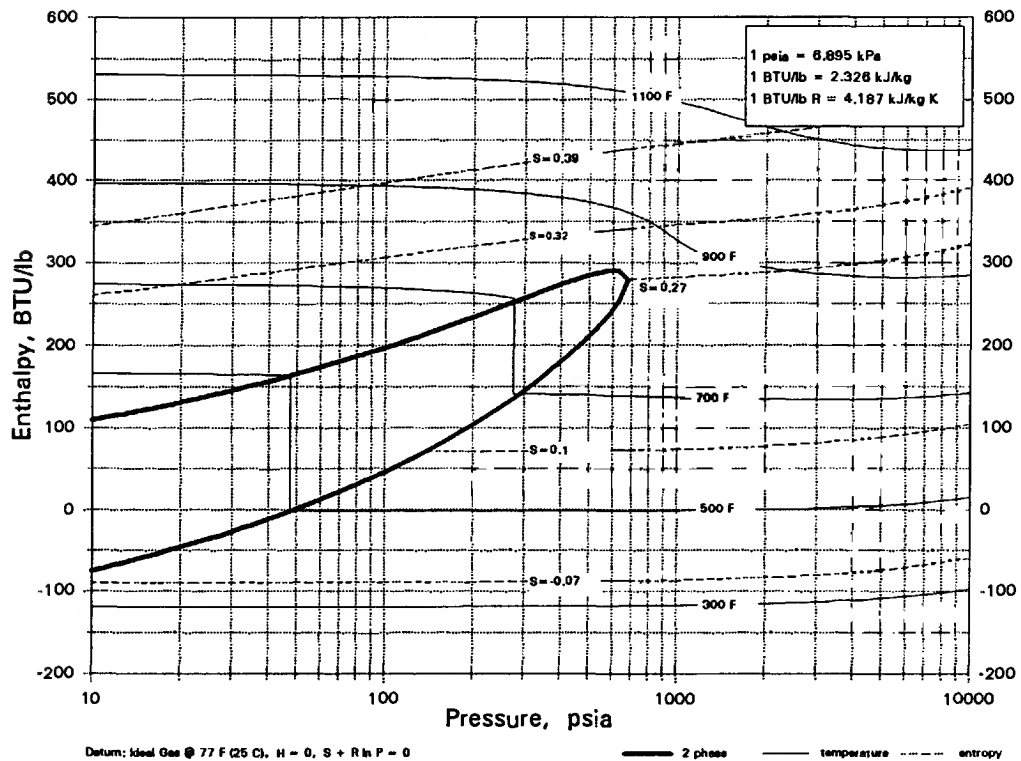
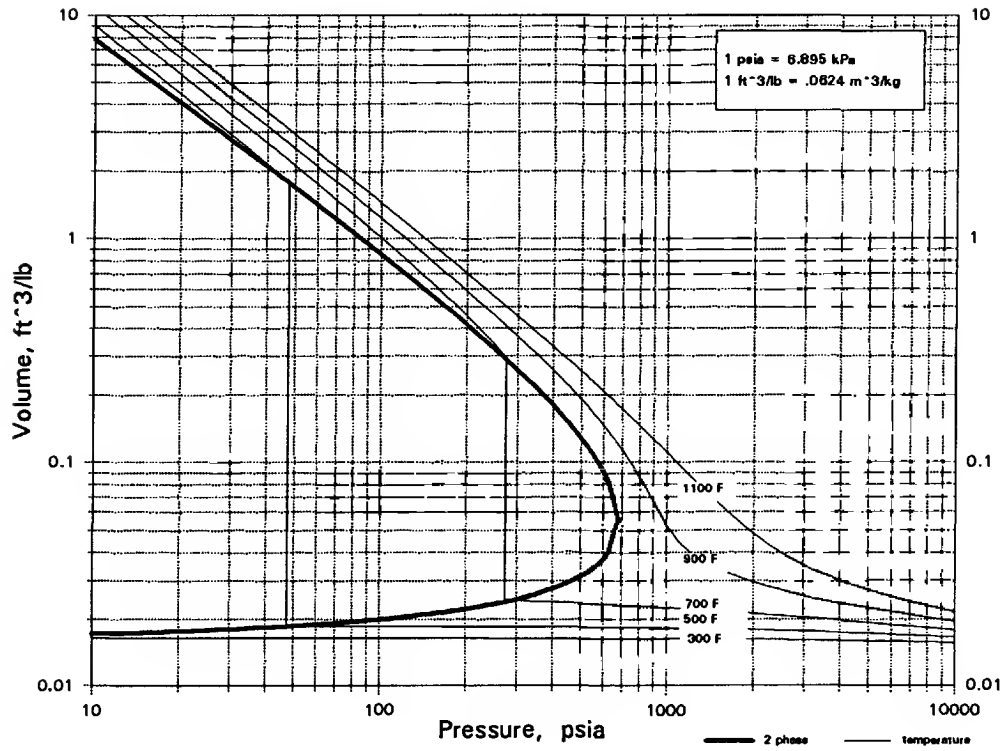


C6H11NO
epsilon-CAPROLACTAM



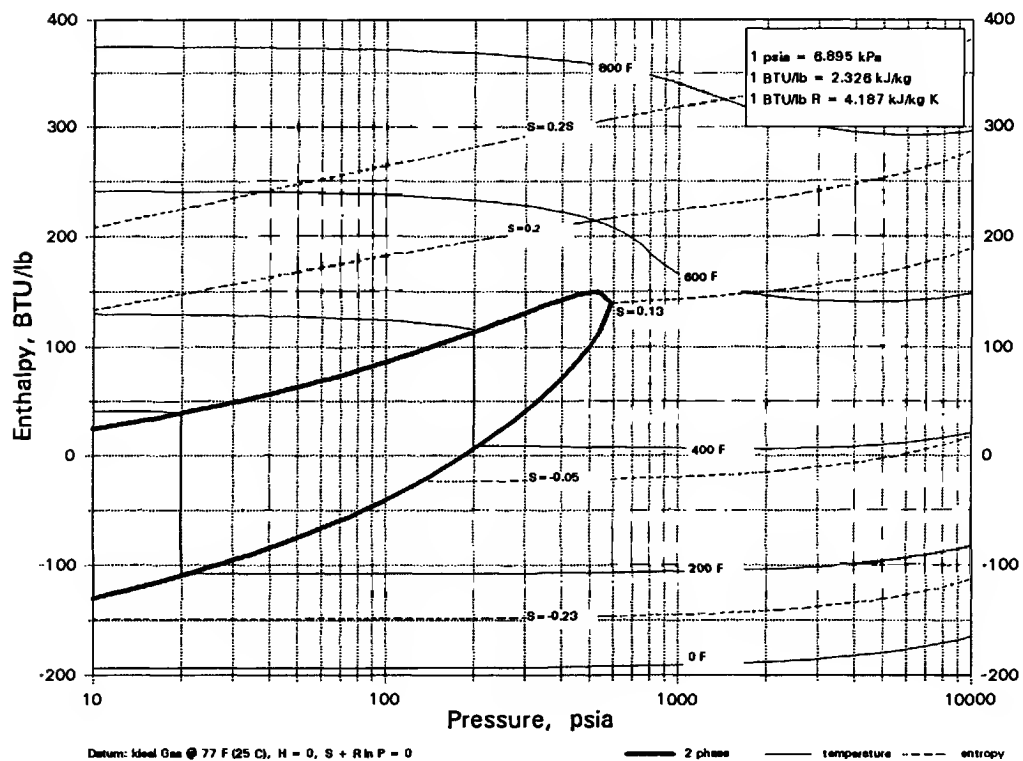
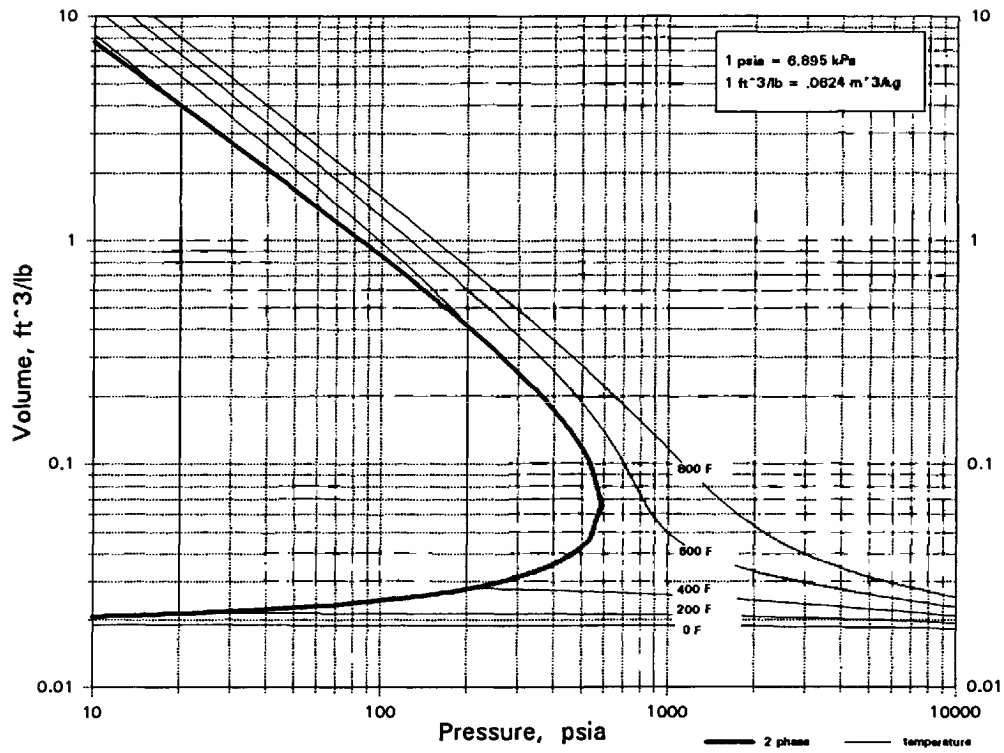
C6H11NO

CYCLOHEXANONE OXIME



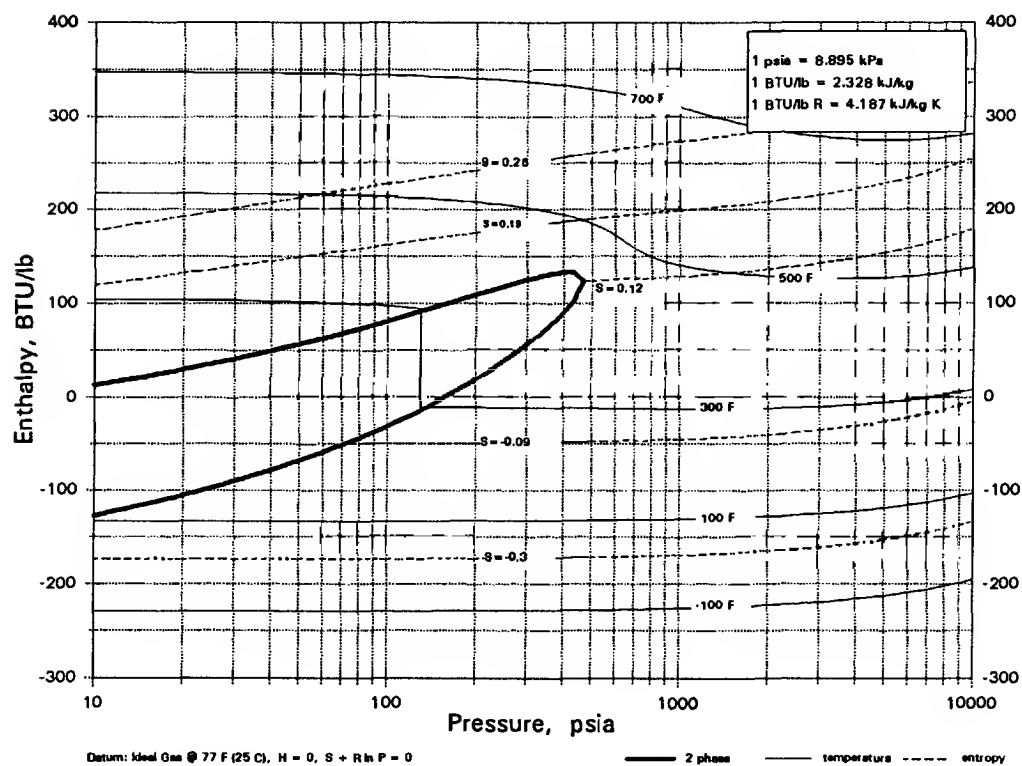
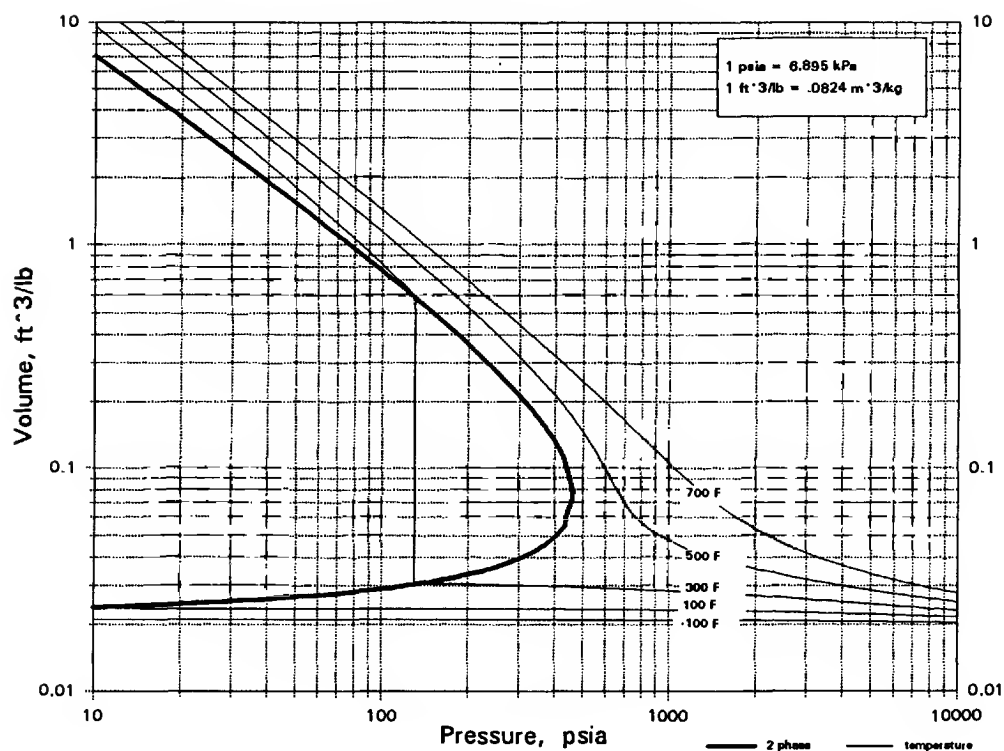
C6H12

CYCLOHEXANE



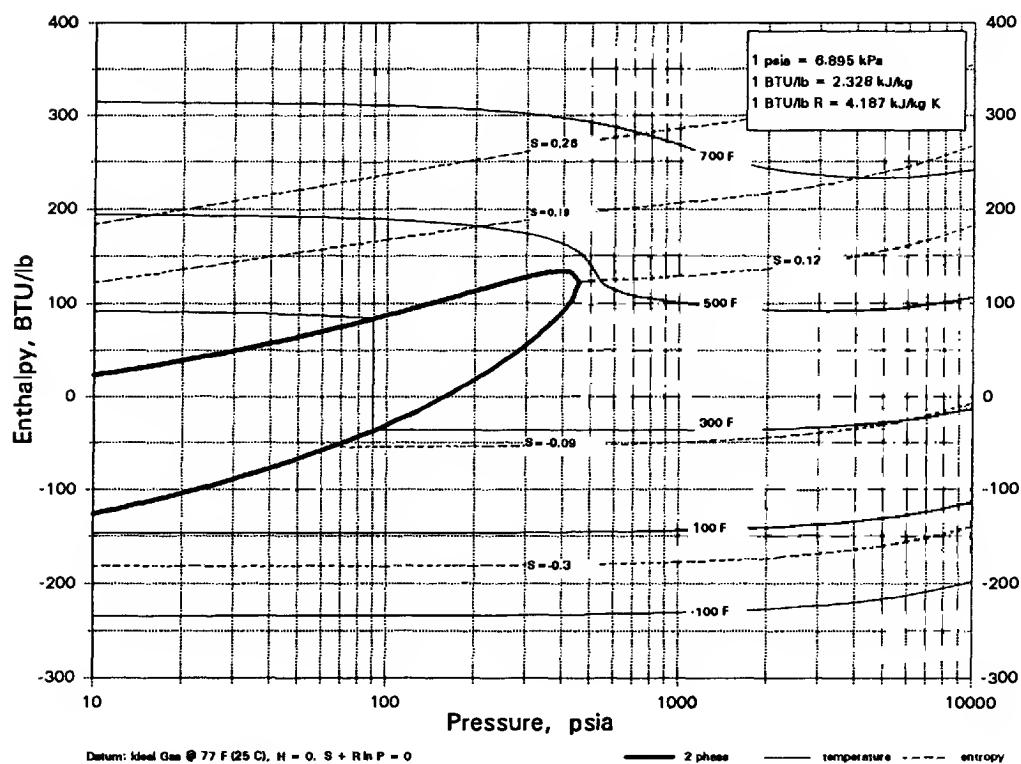
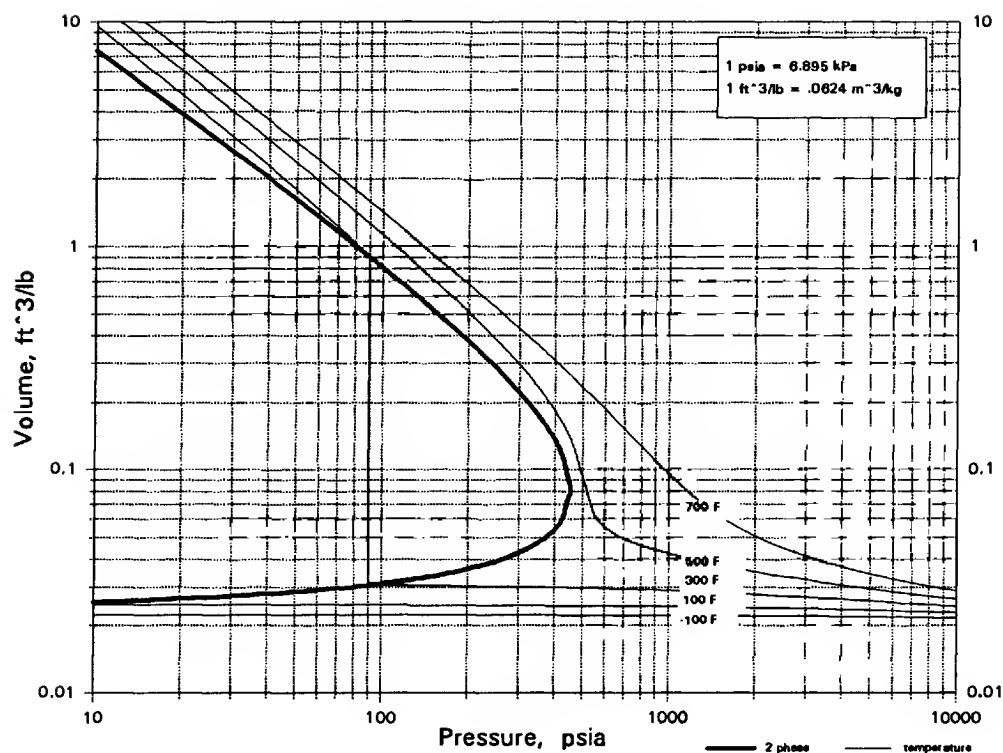
C6H12

2-3-DIMETHYL-1-BUTENE



C6H12

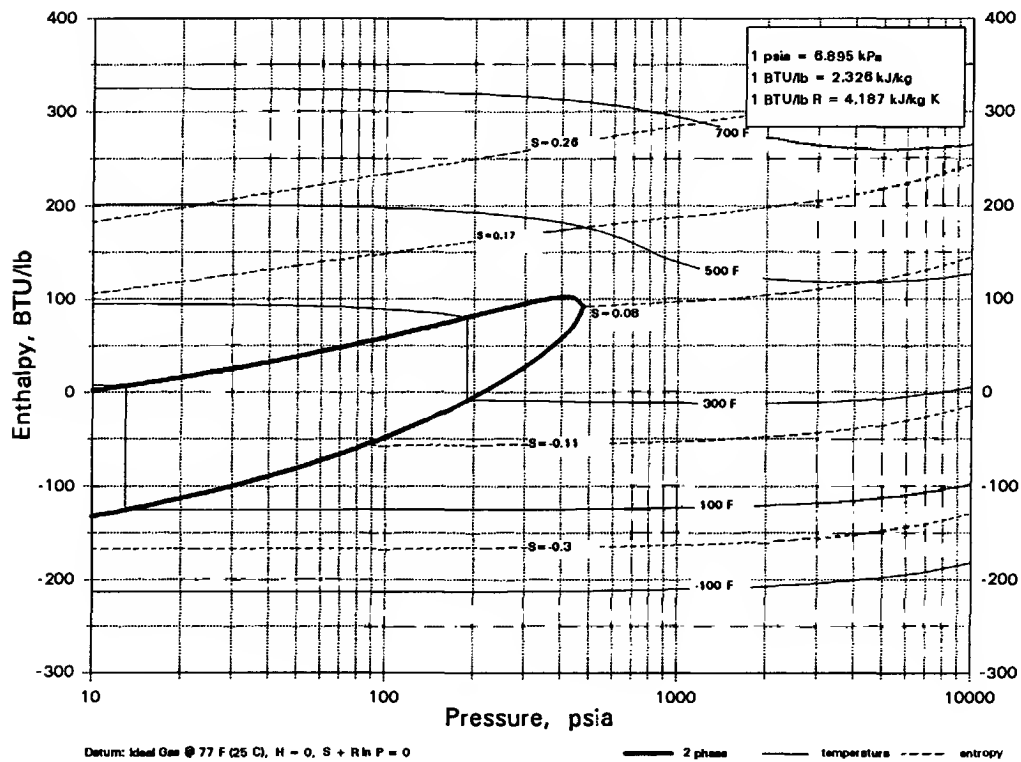
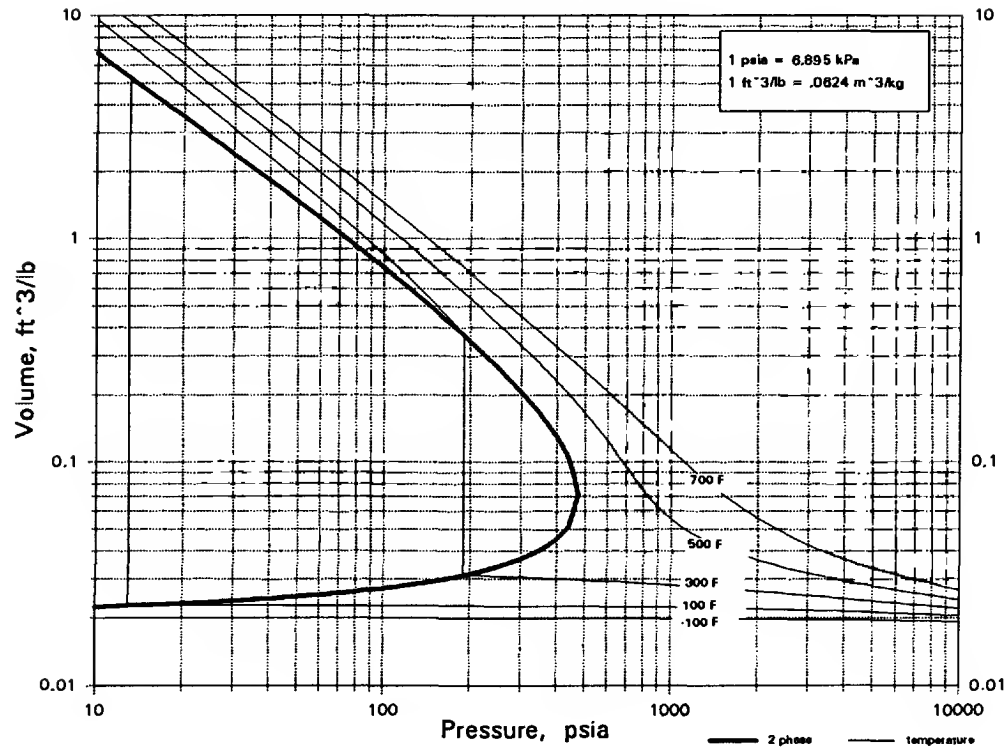
2-3-DIMETHYL-2-BUTENE



Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

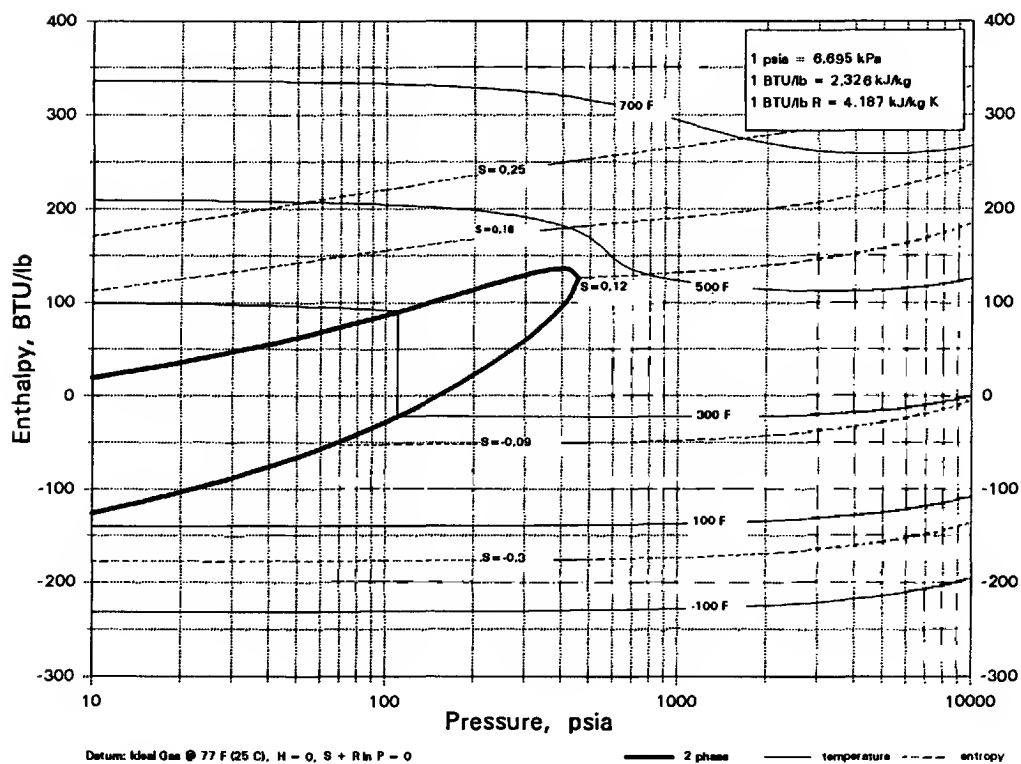
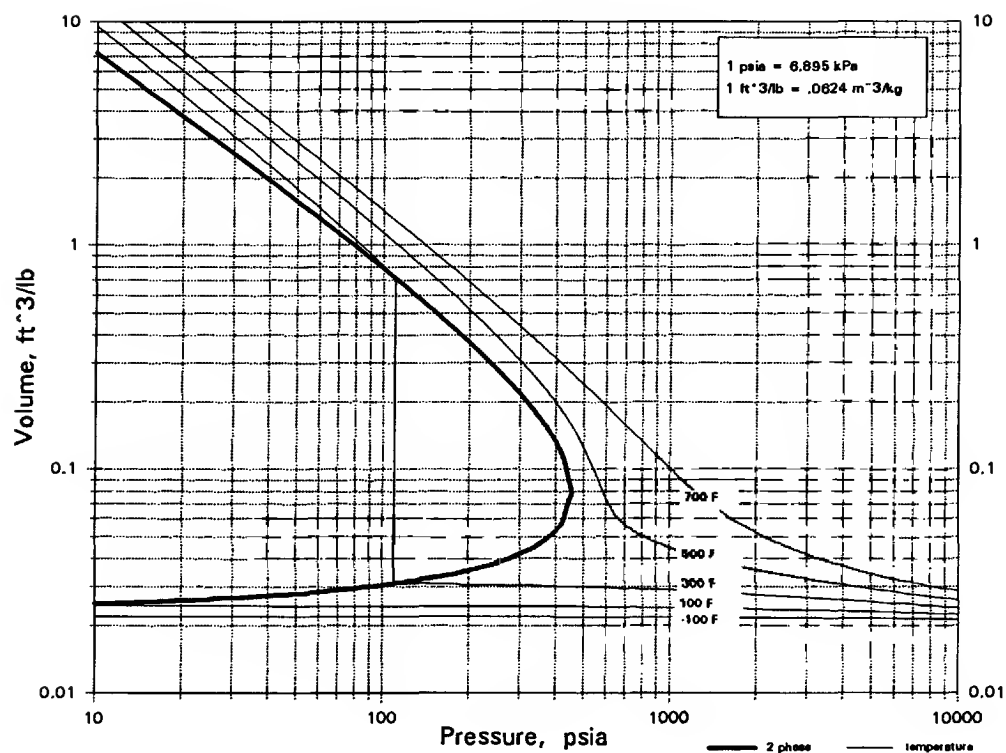
C6H12

3-3-DIMETHYL-1-BUTENE



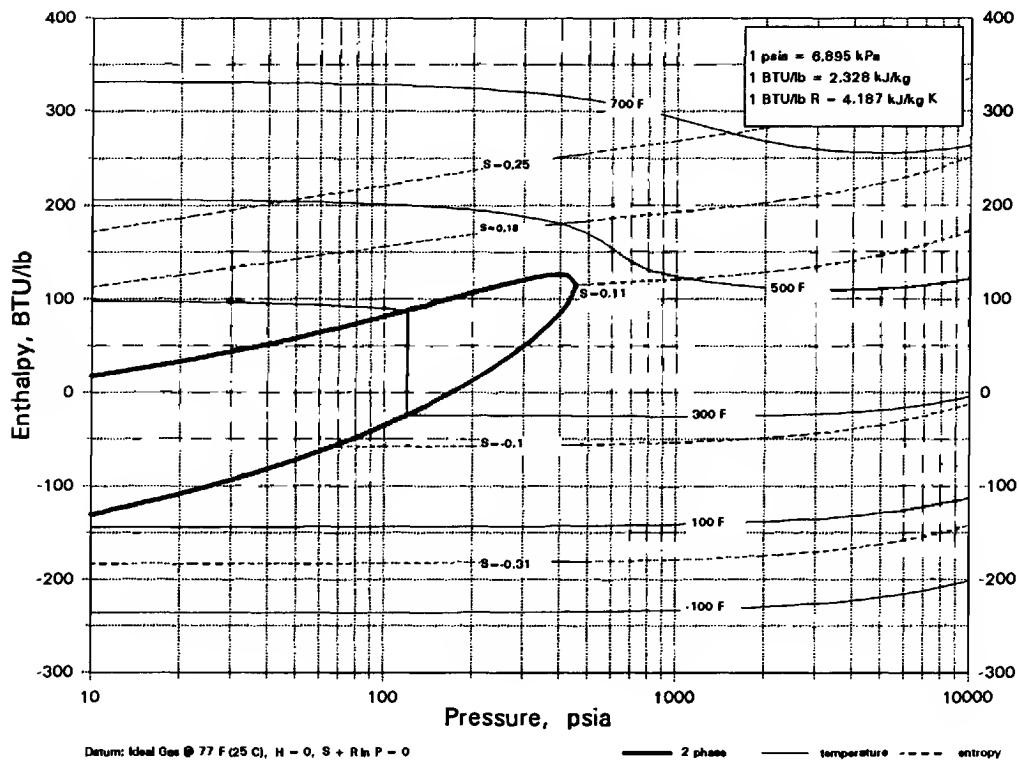
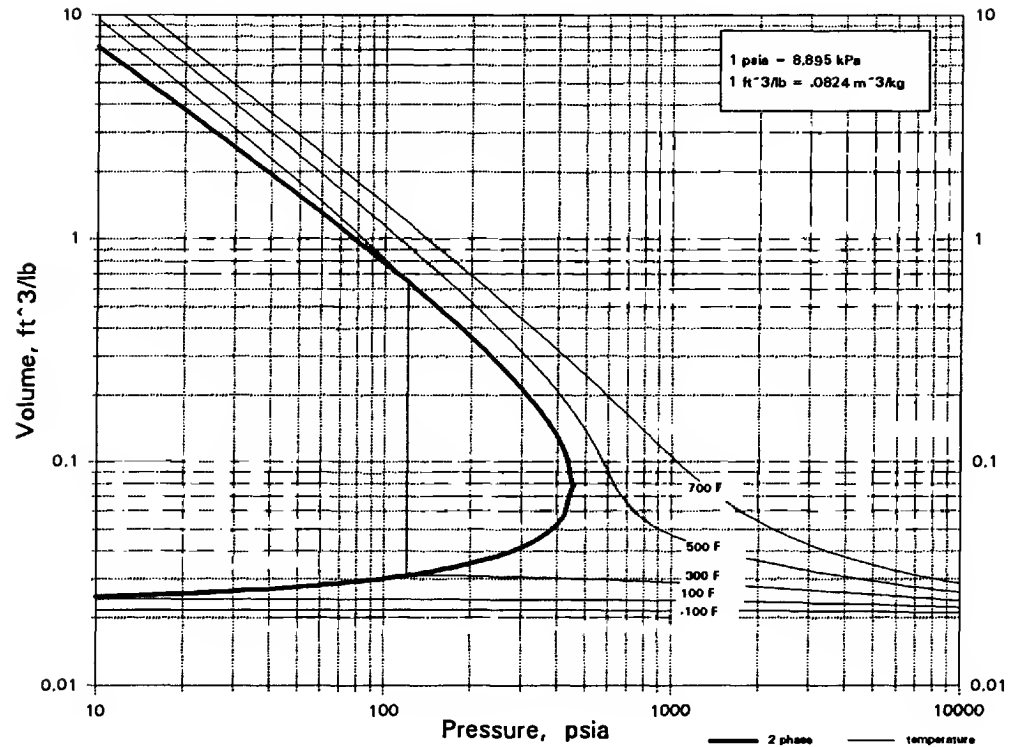
C6H12

2-ETHYL-1-BUTENE



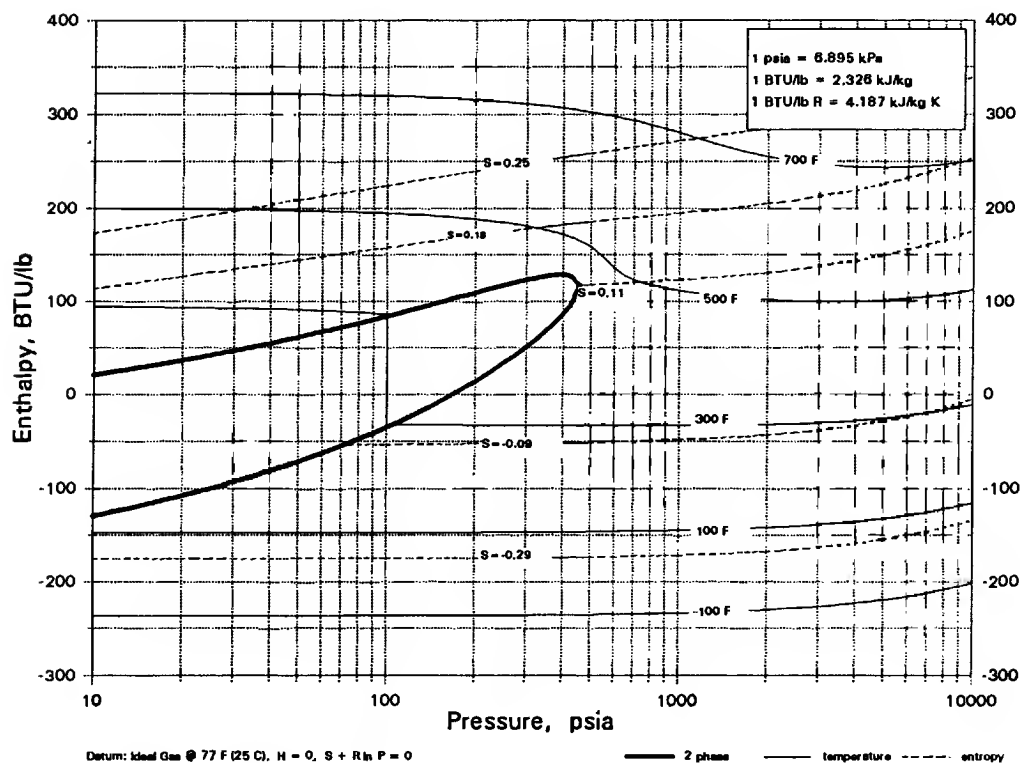
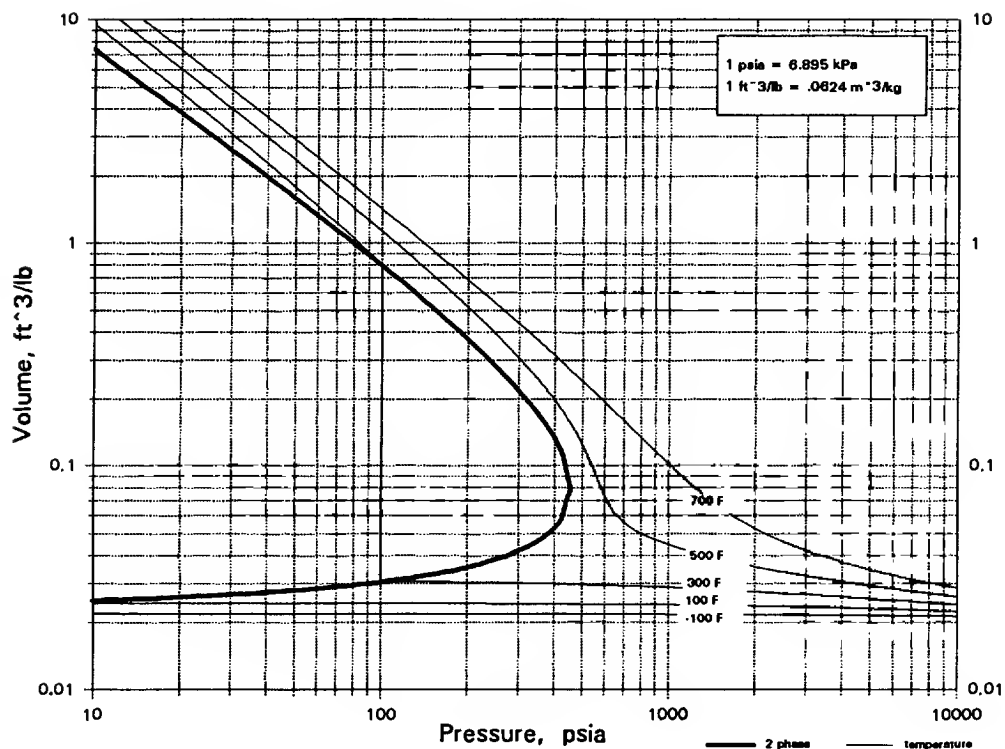
C6H12

1-HEXENE



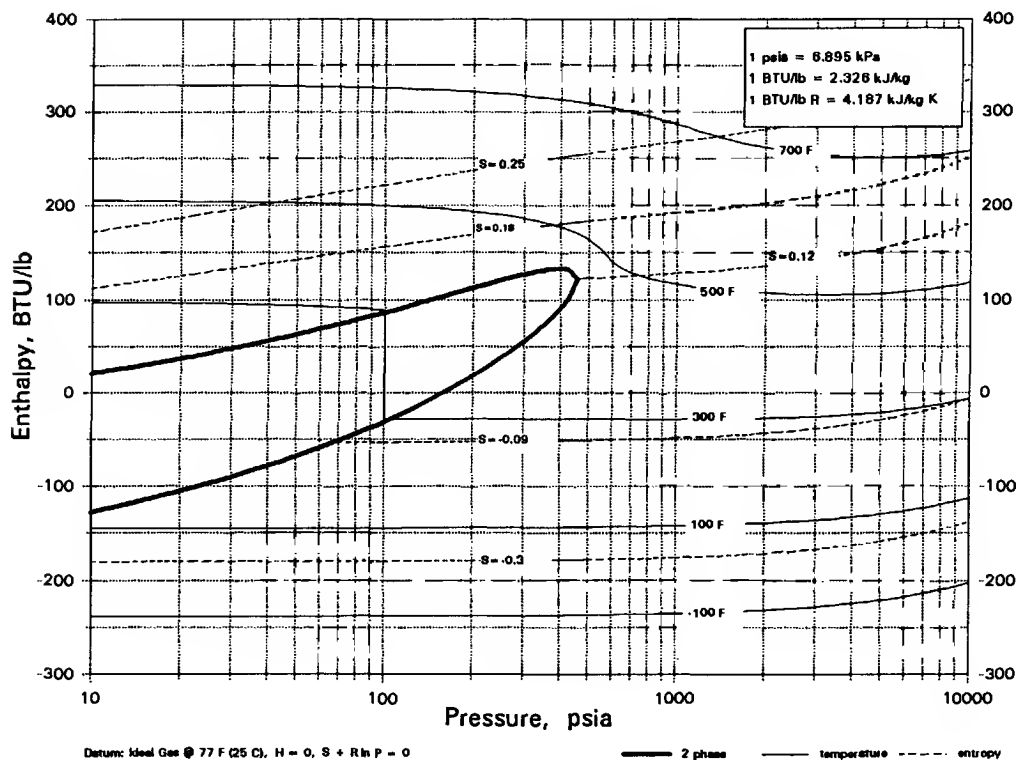
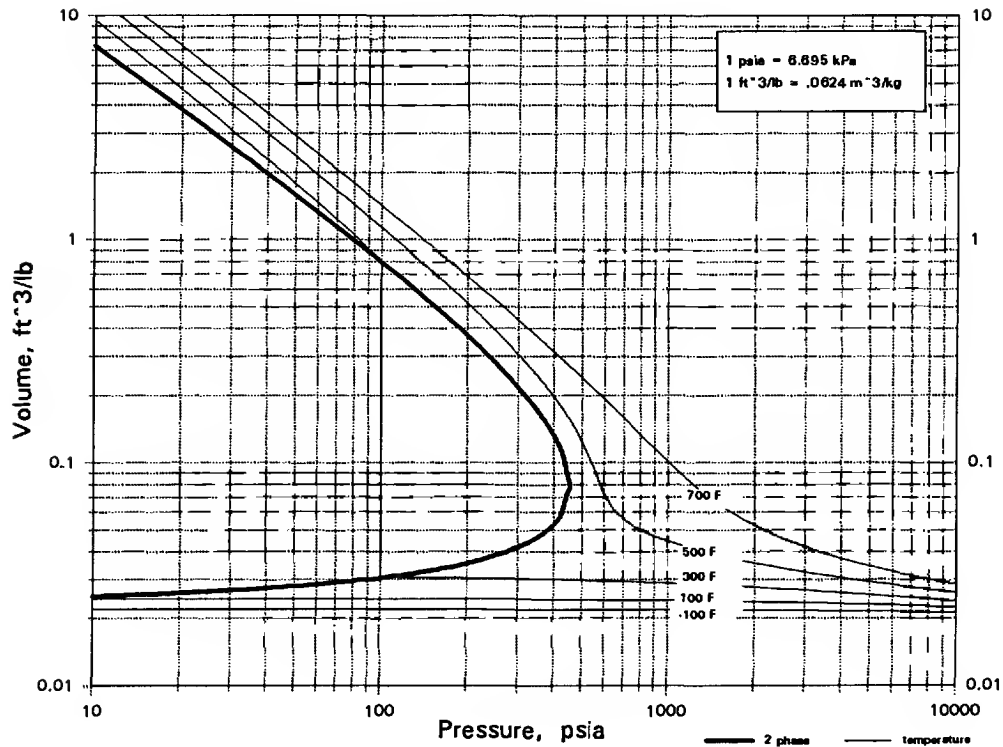
C6H12

cis-2-HEXENE



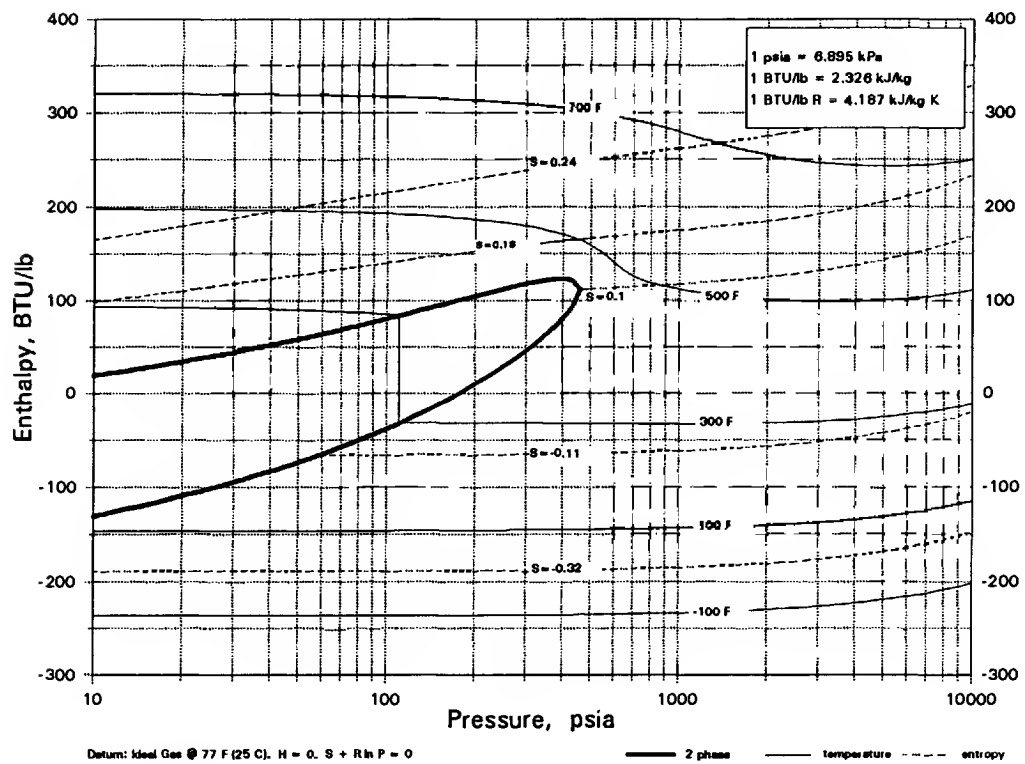
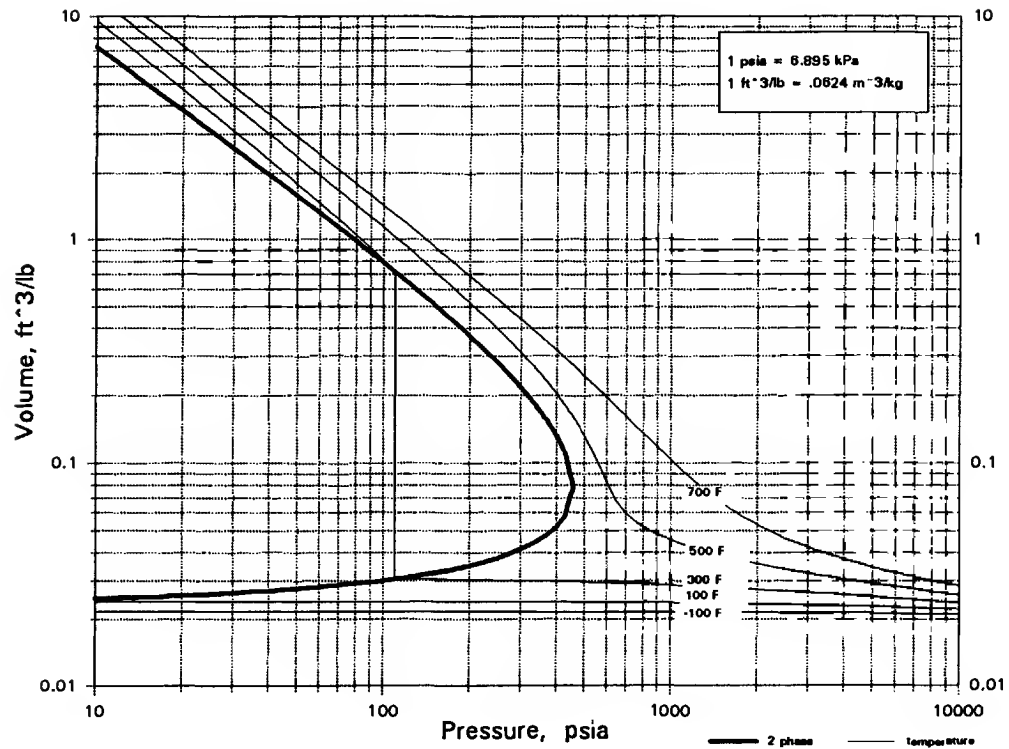
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trans-2-HEXENE



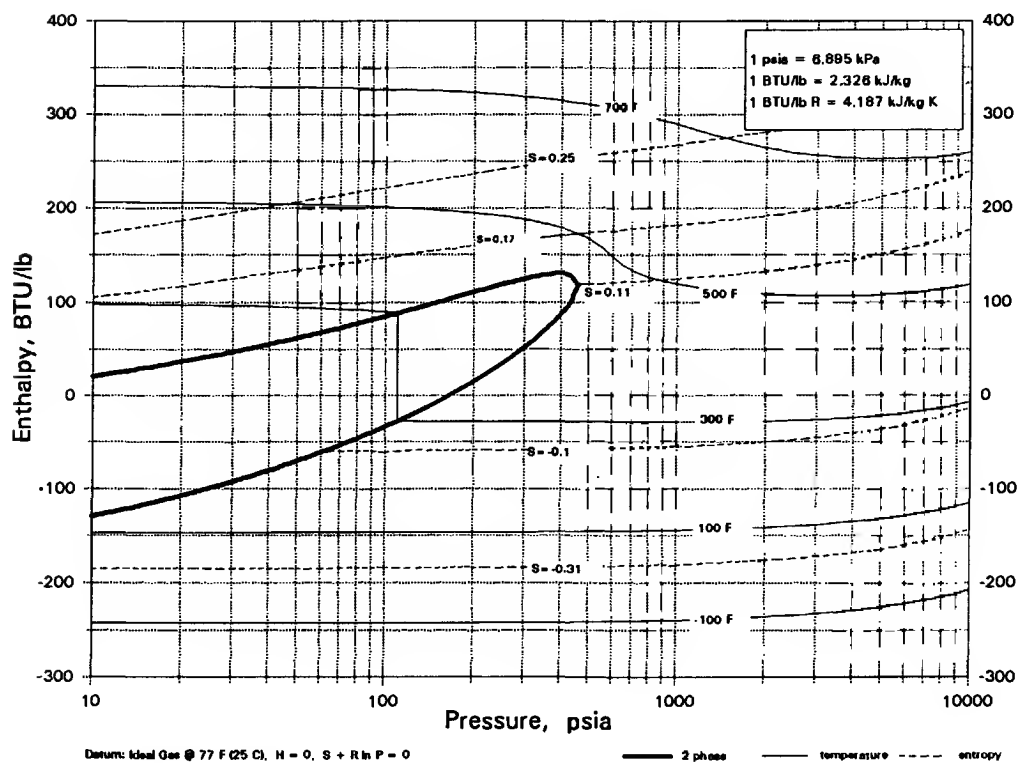
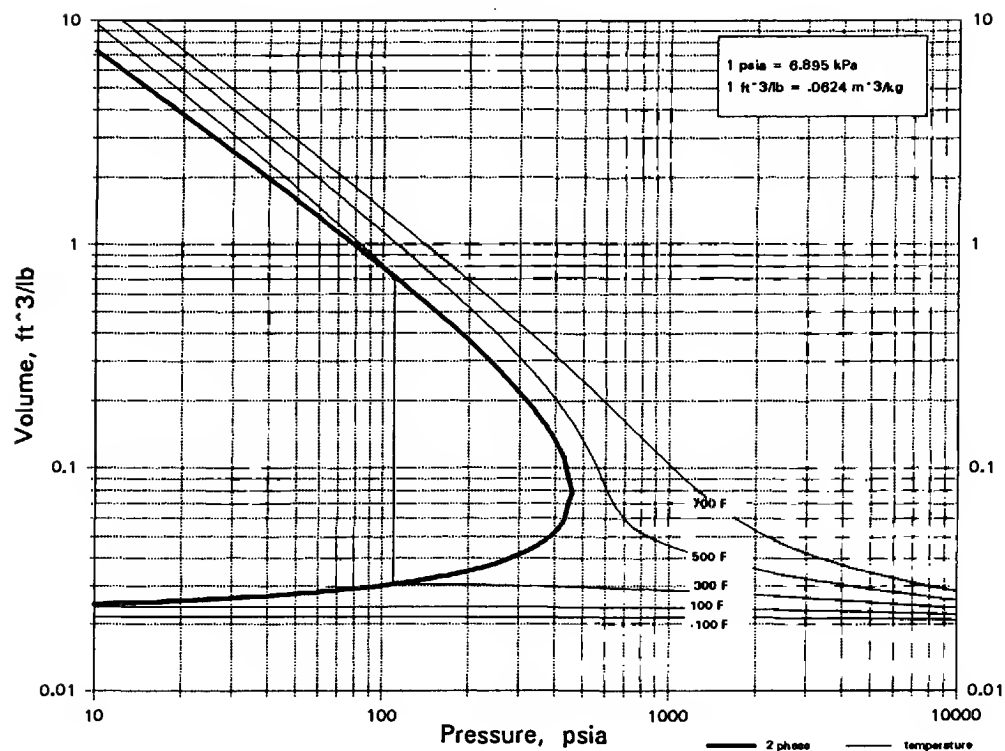
C6H12

cis-3-HEXENE



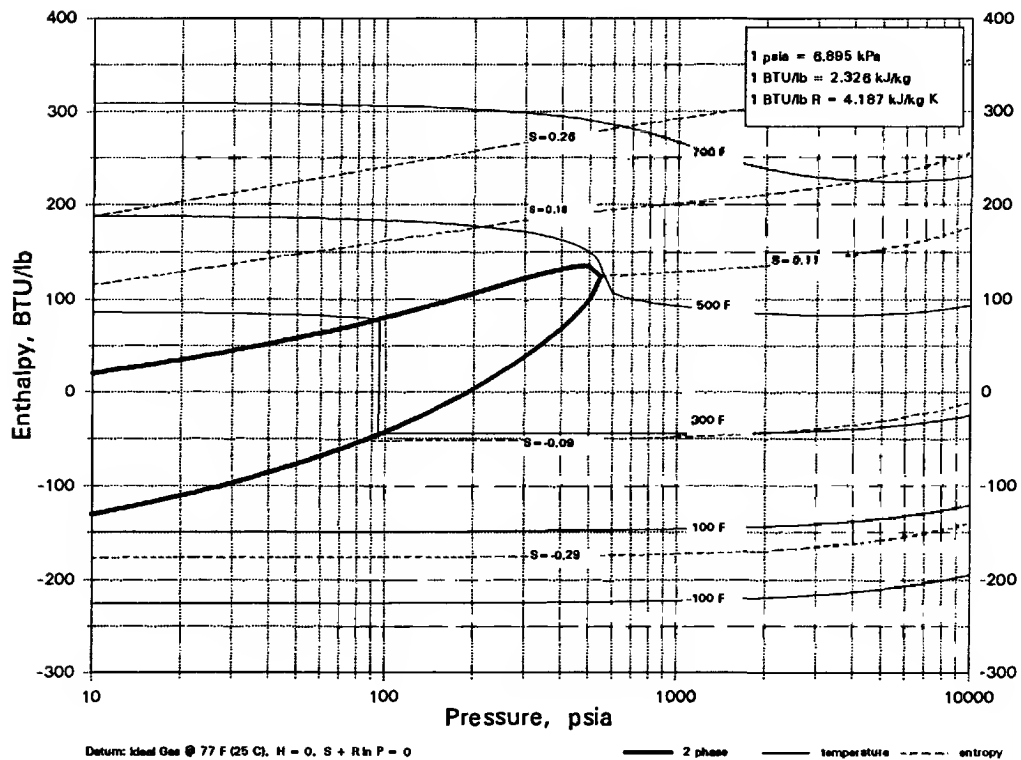
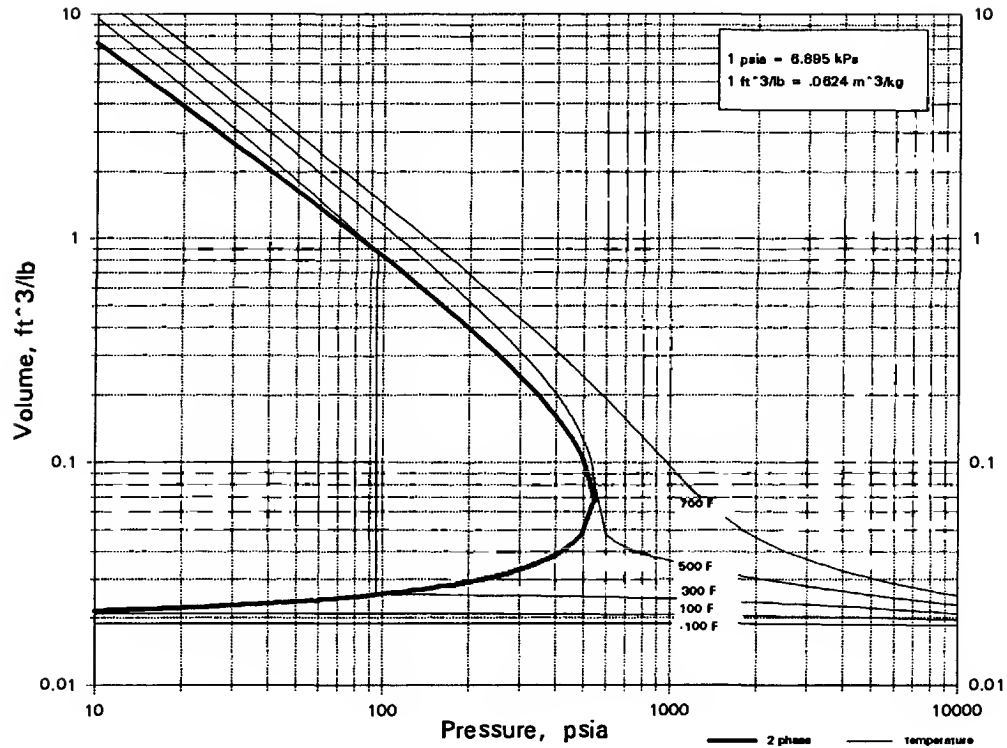
C6H12

trans-3-HEXENE



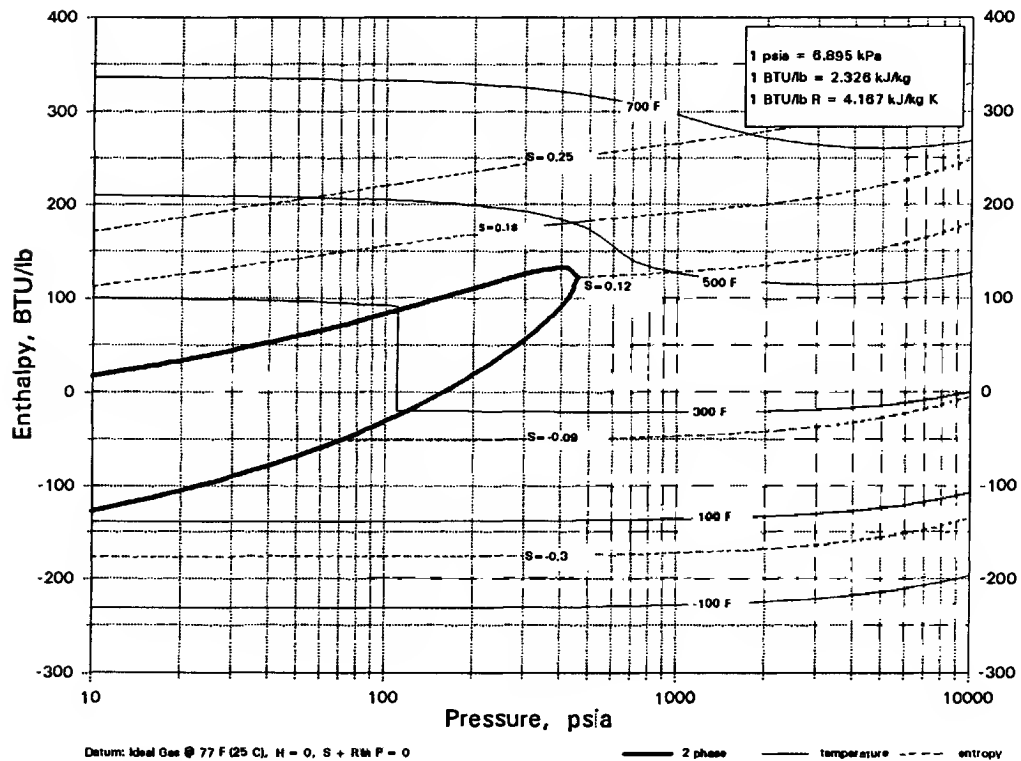
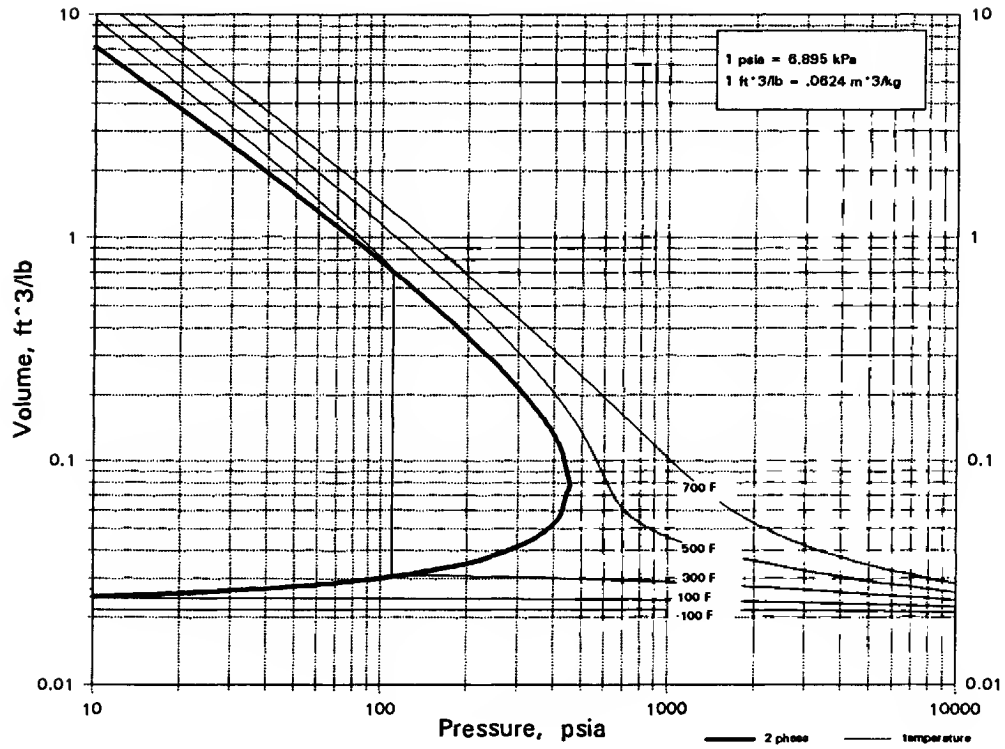
C6H12

METHYLCYCLOPENTANE



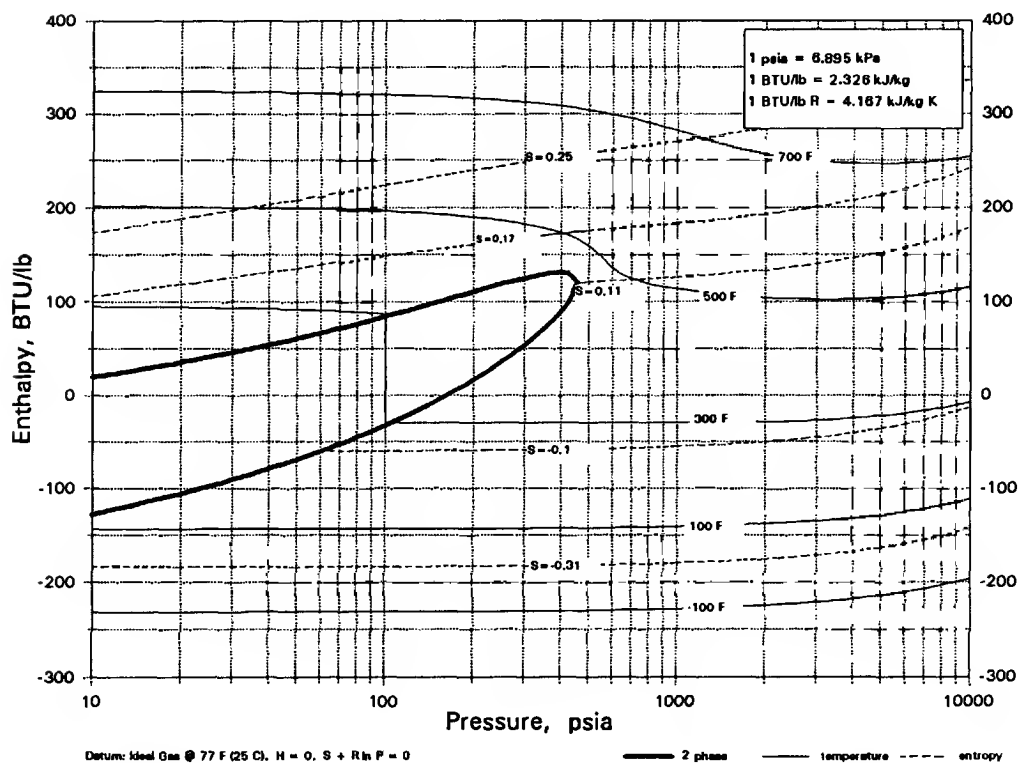
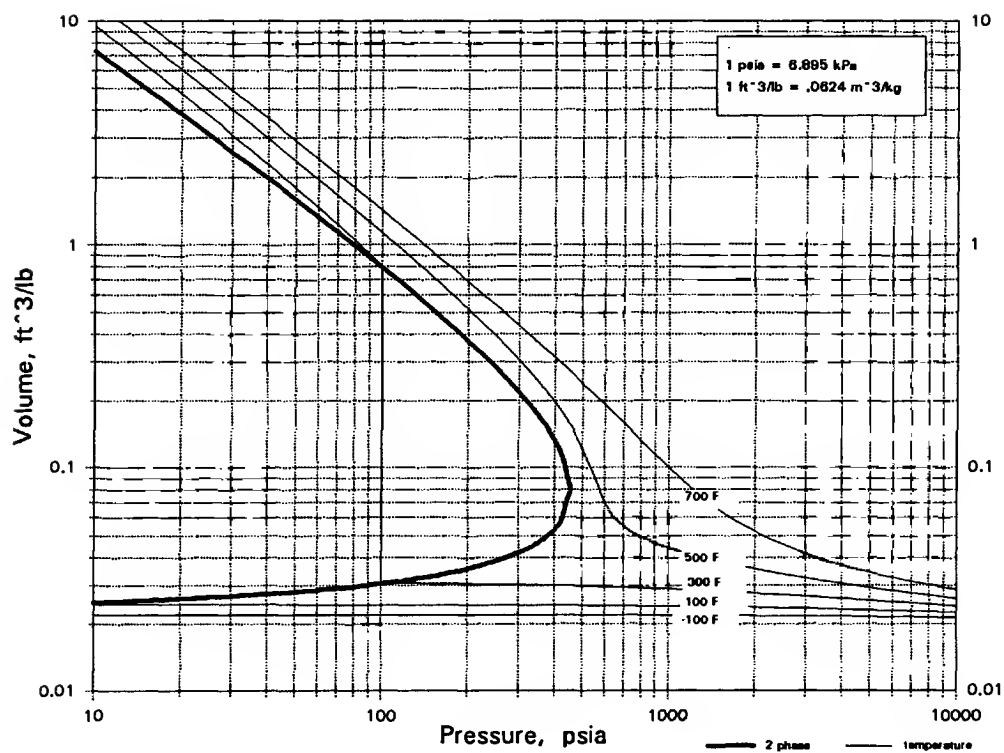
C6H12

2-METHYL-1-PENTENE



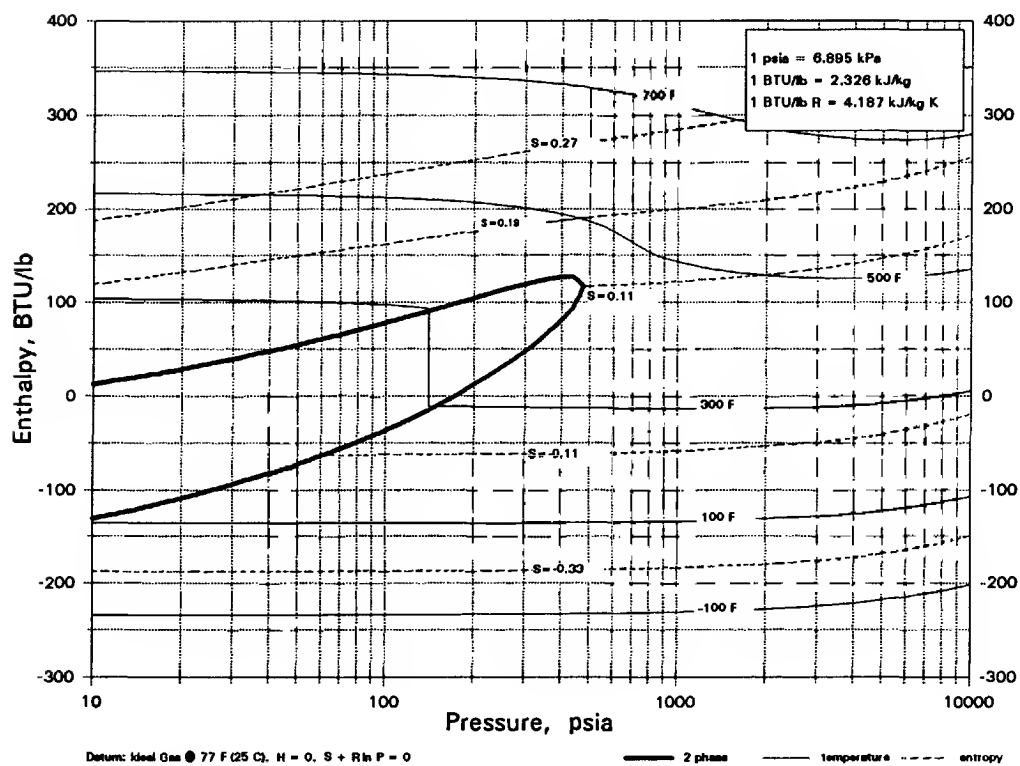
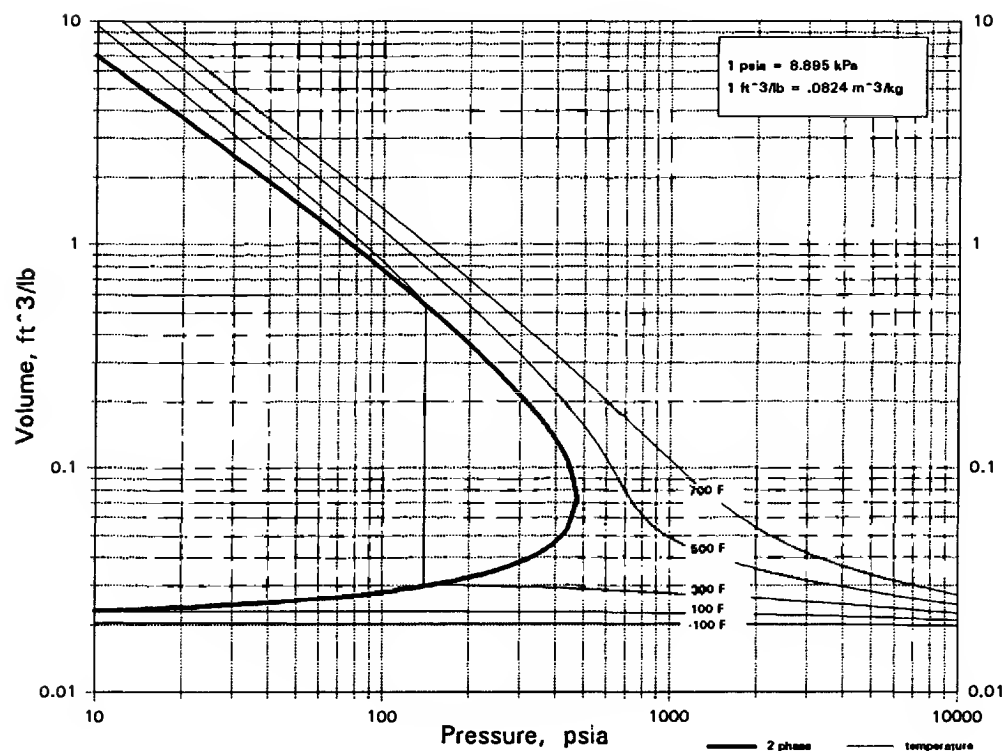
C6H12

2-METHYL-2-PENTENE



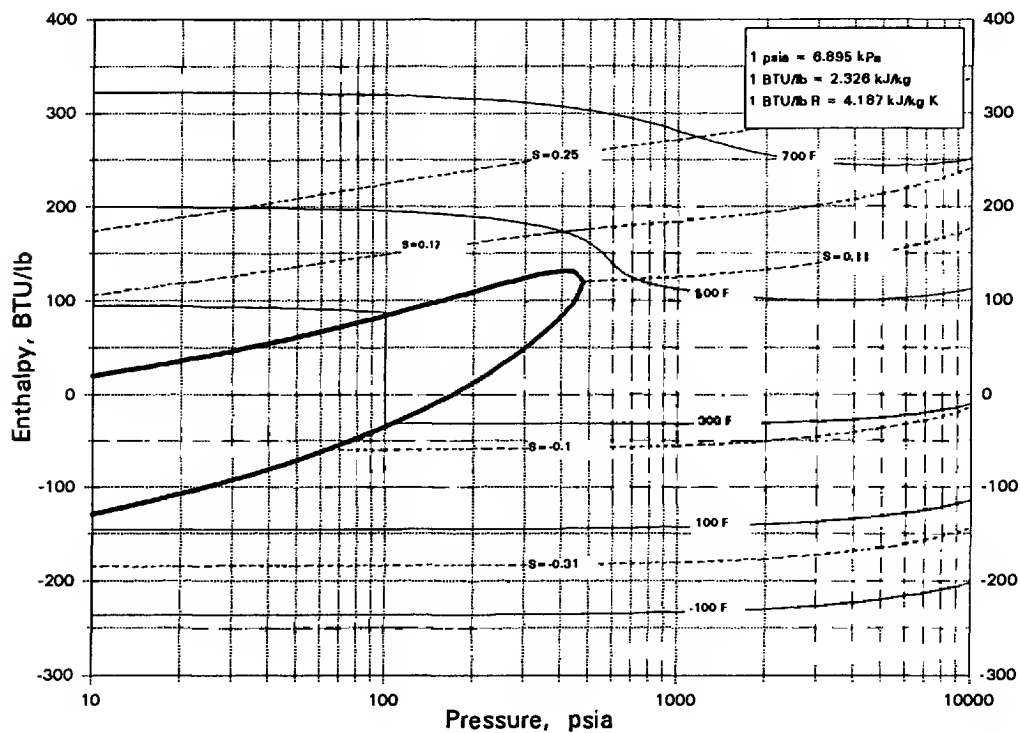
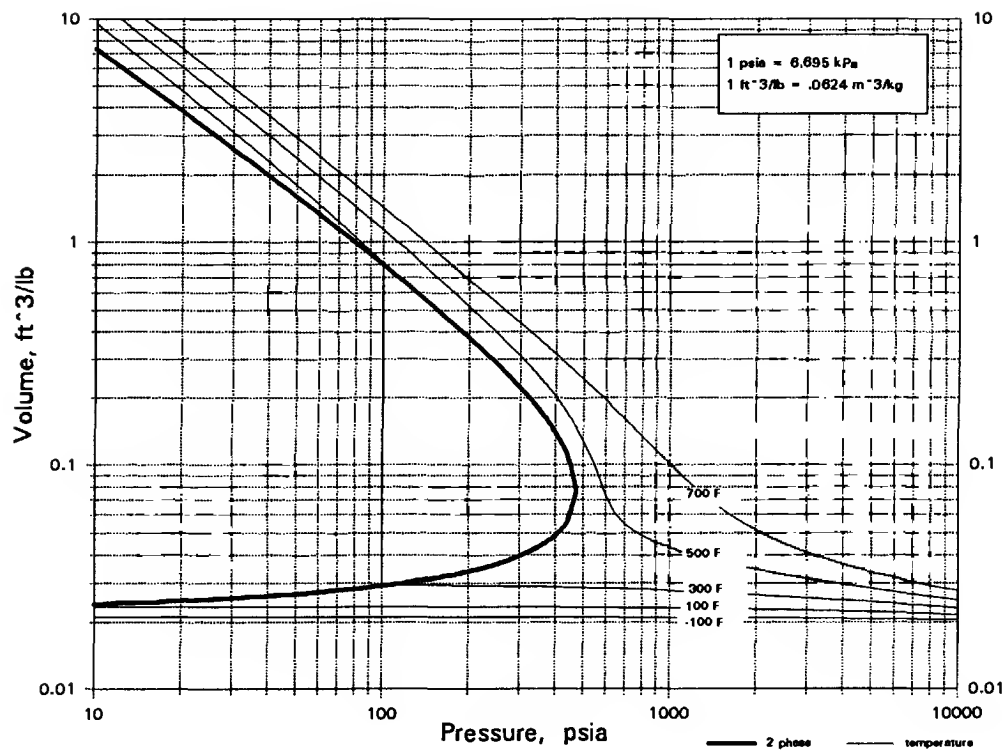
C6H12

3-METHYL-1-PENTENE



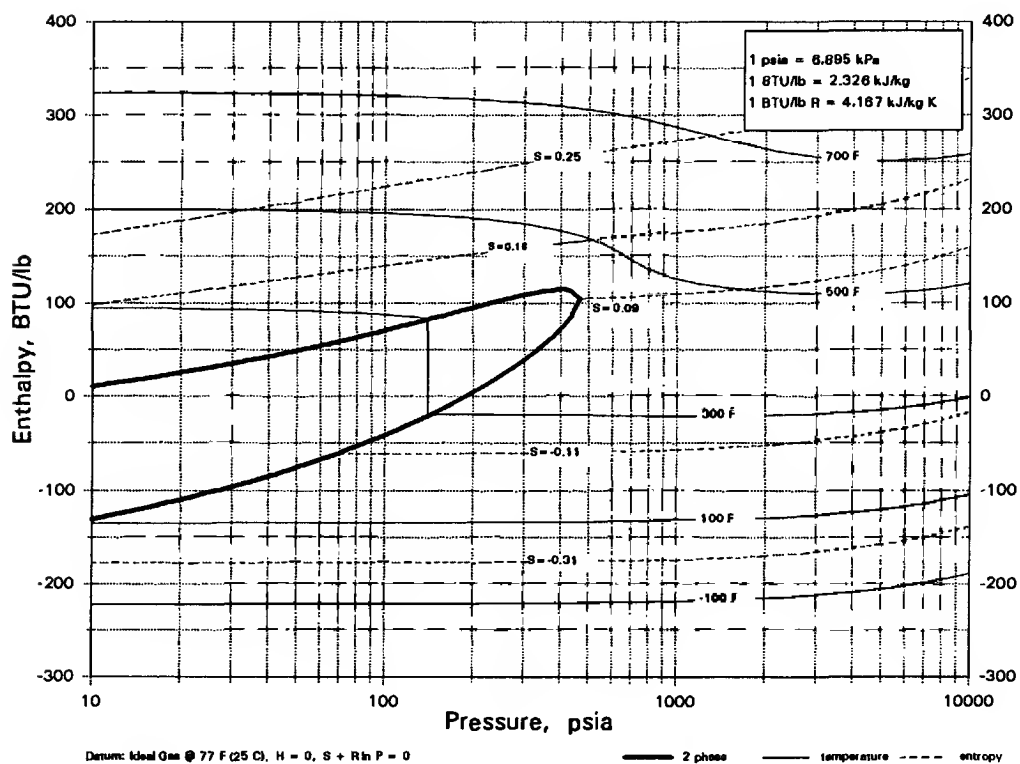
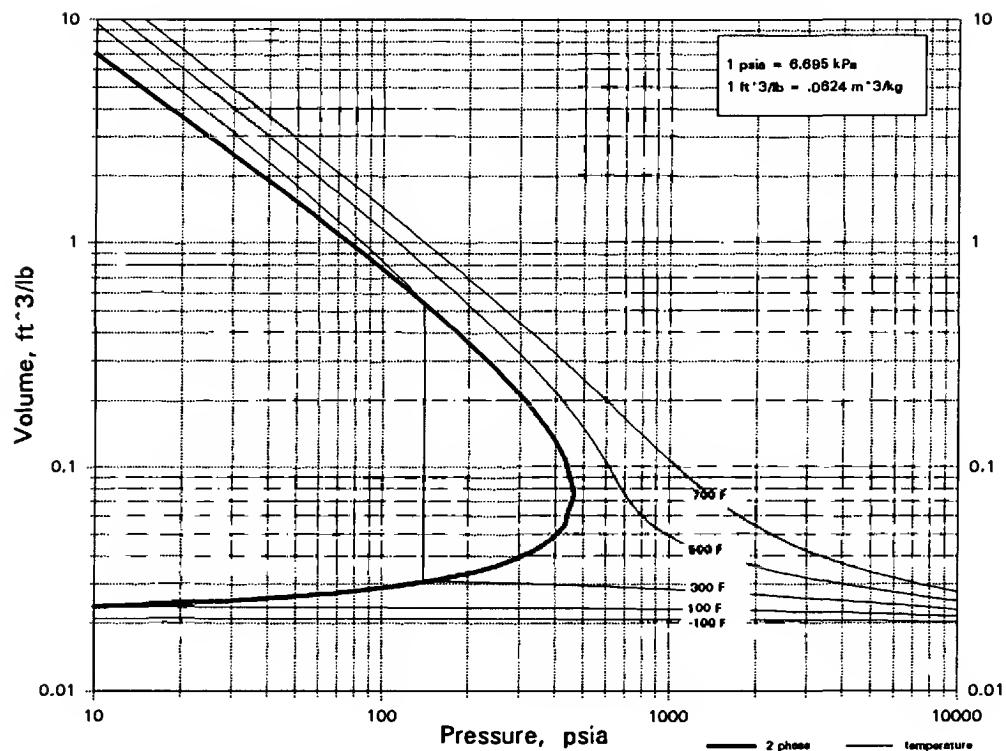
C6H12

3-METHYL-cis-2-PENTENE

Datum: Ideal Gas @ 77 F (25 C), $H = 0$, $S + R \ln P = 0$

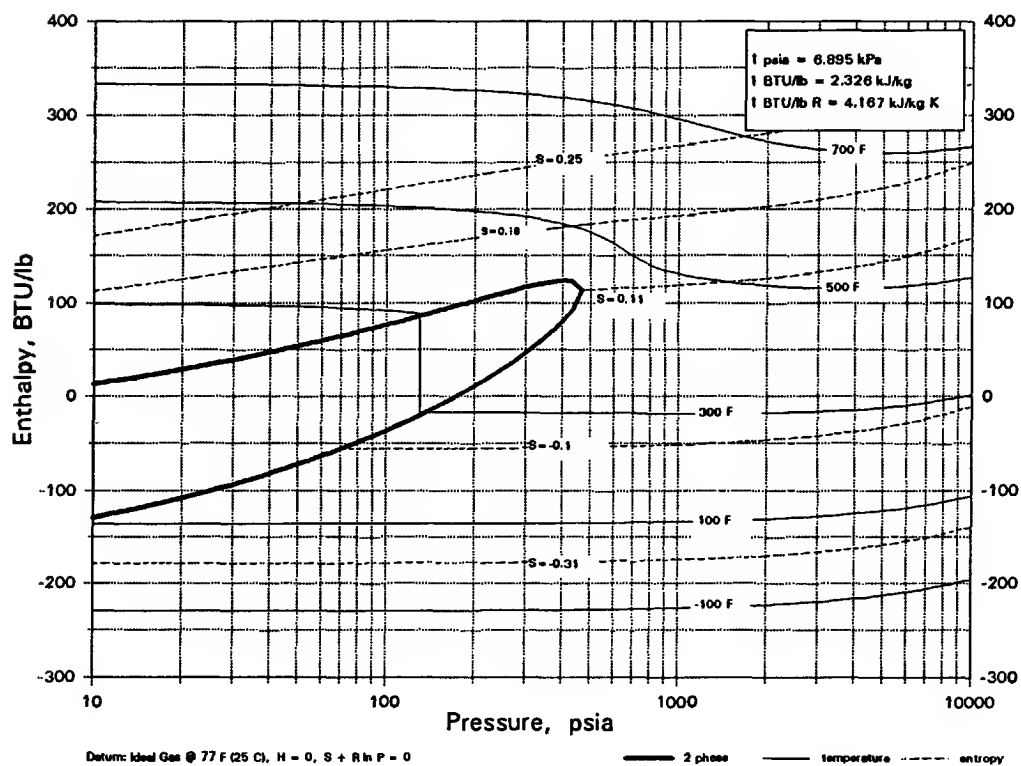
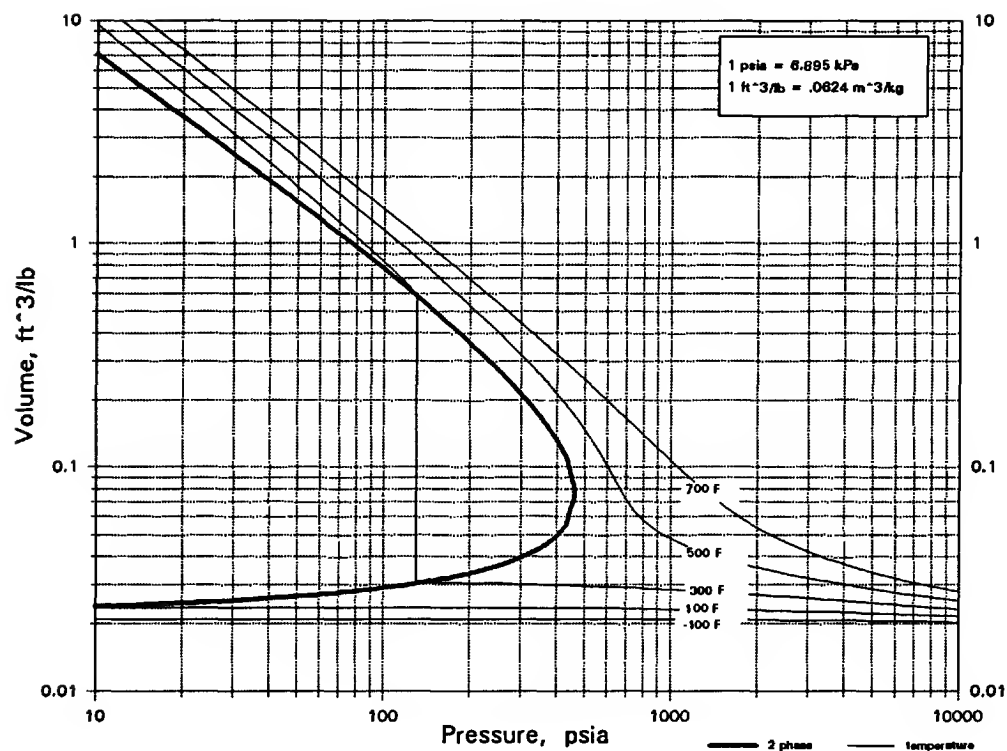
C6H12

4-METHYL-1-PENTENE



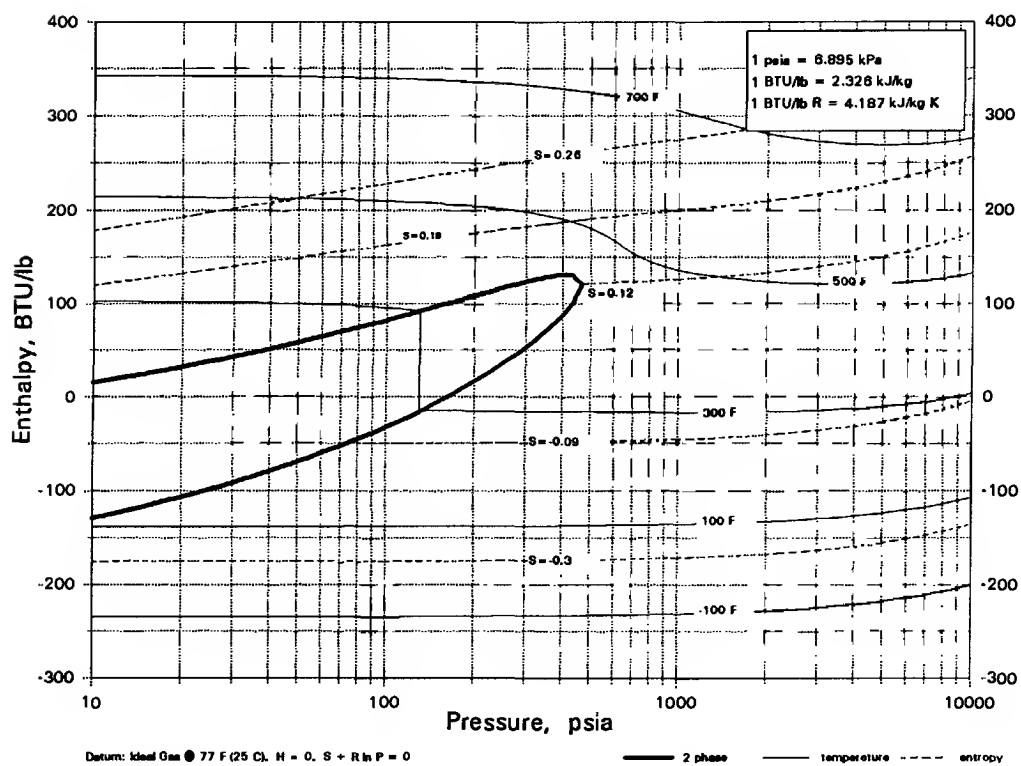
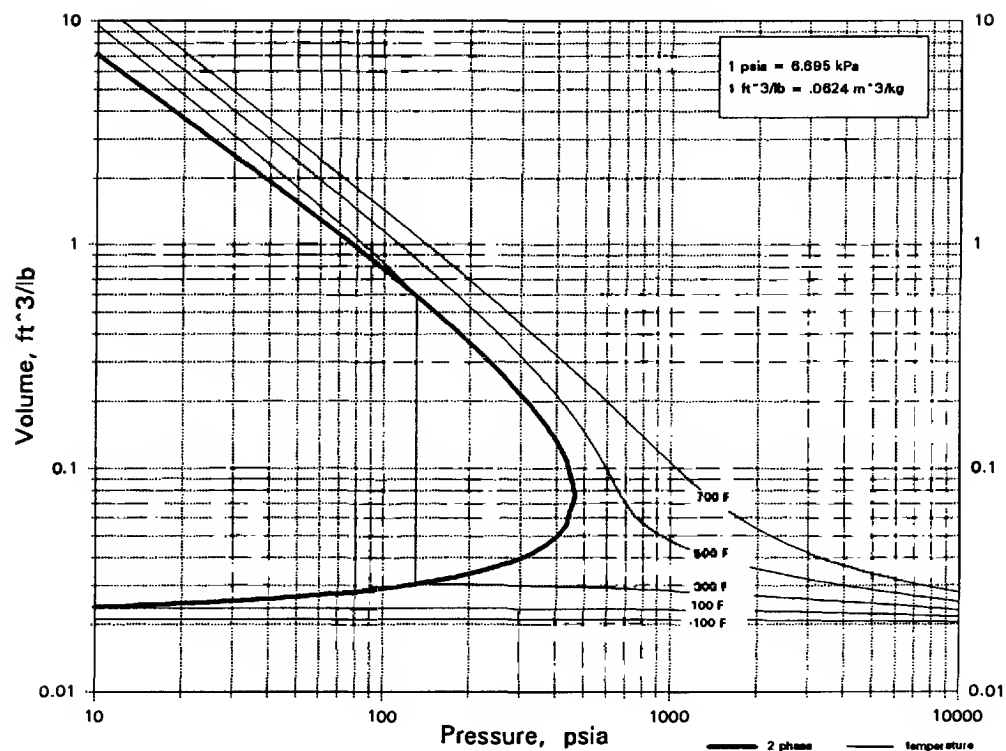
C6H12

4-METHYL-cis-2-PENTENE



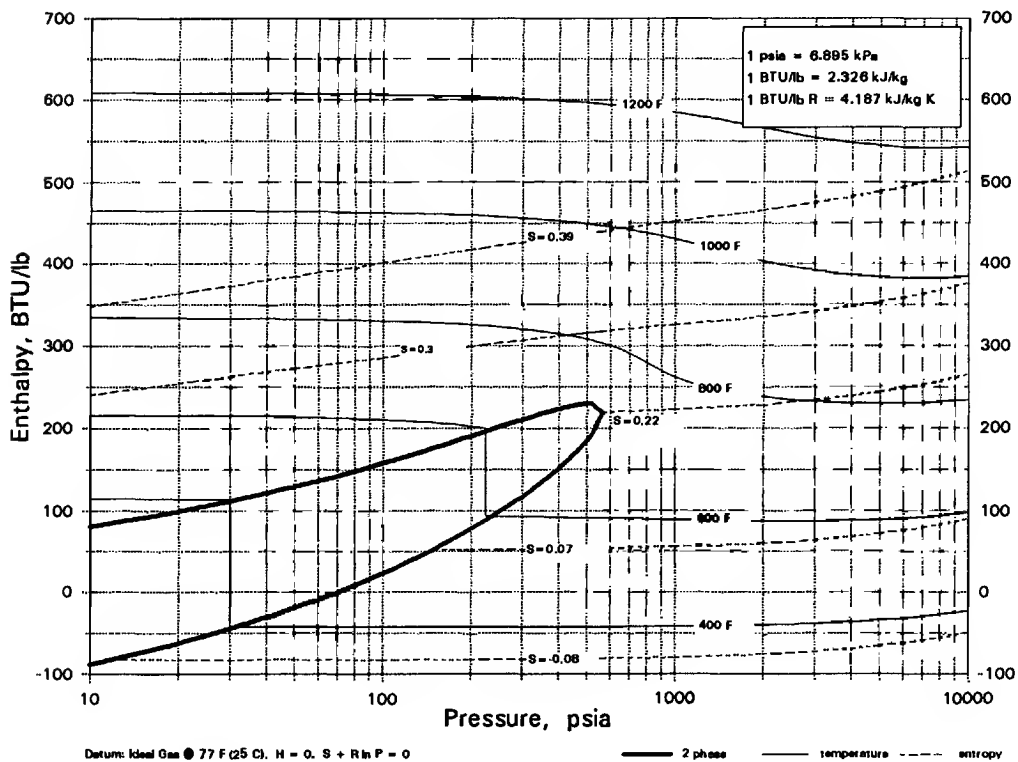
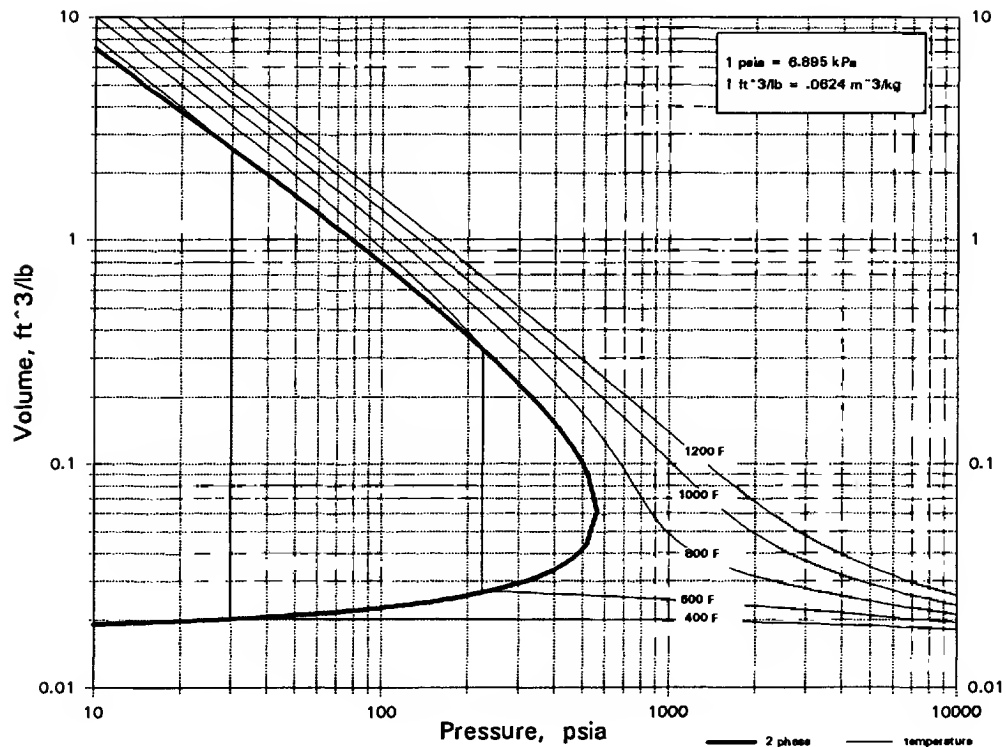
C6H12

4-METHYL-trans-2-PENTENE

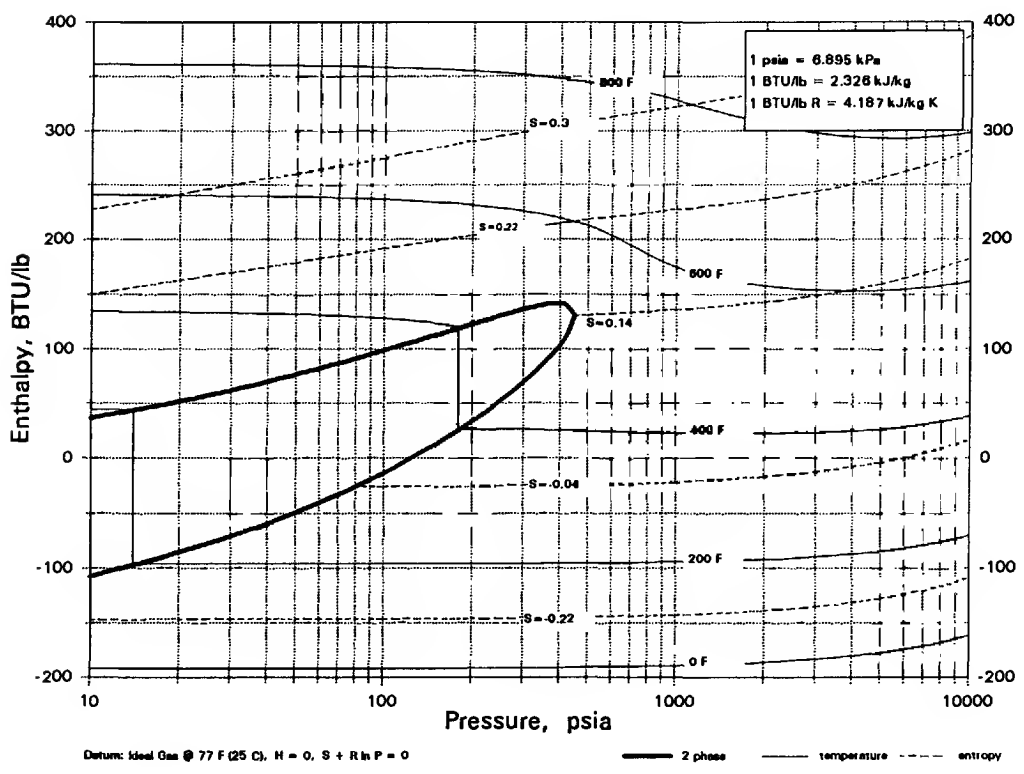
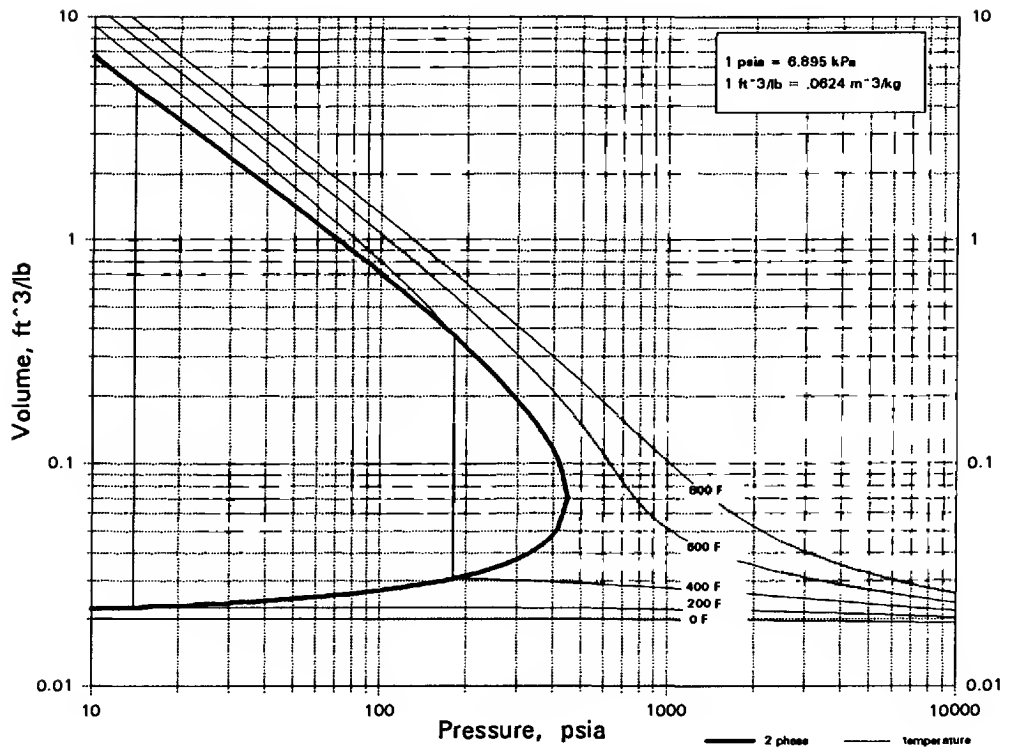


C6H12N2

TRIETHYLENEDIAMINE

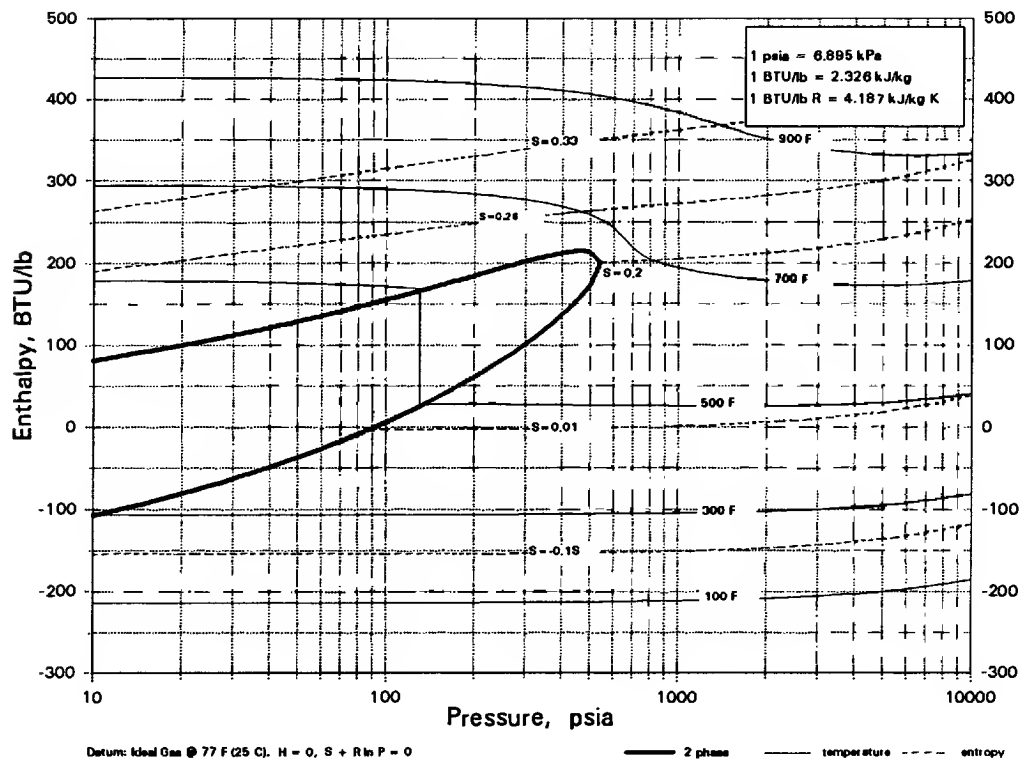
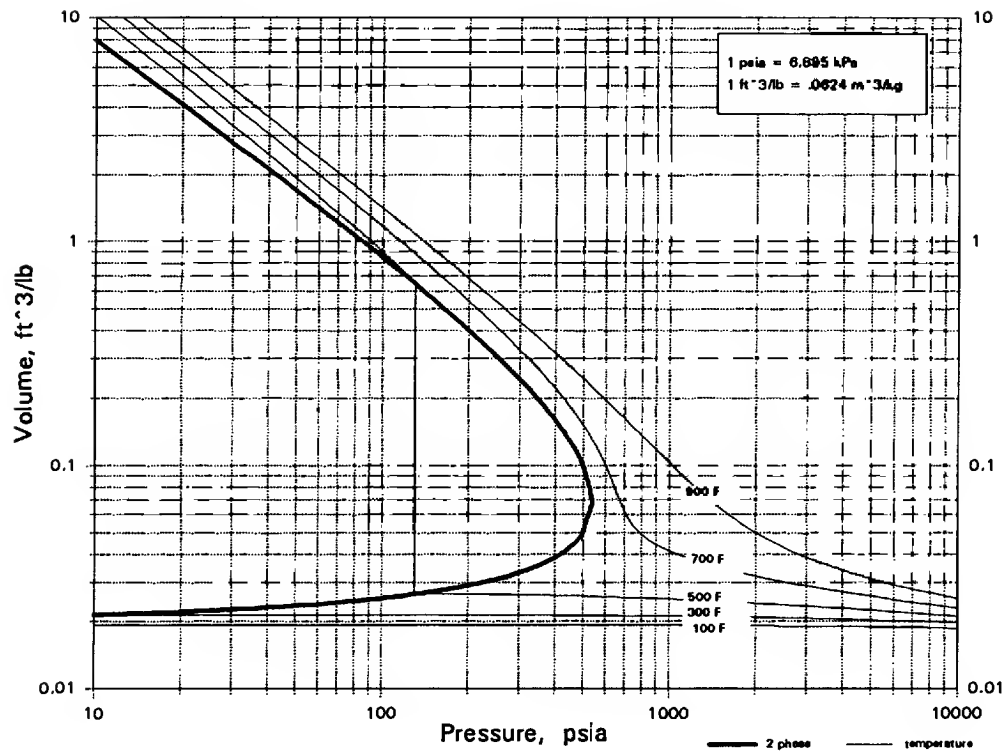


C6H12O
BUTYL VINYL ETHER

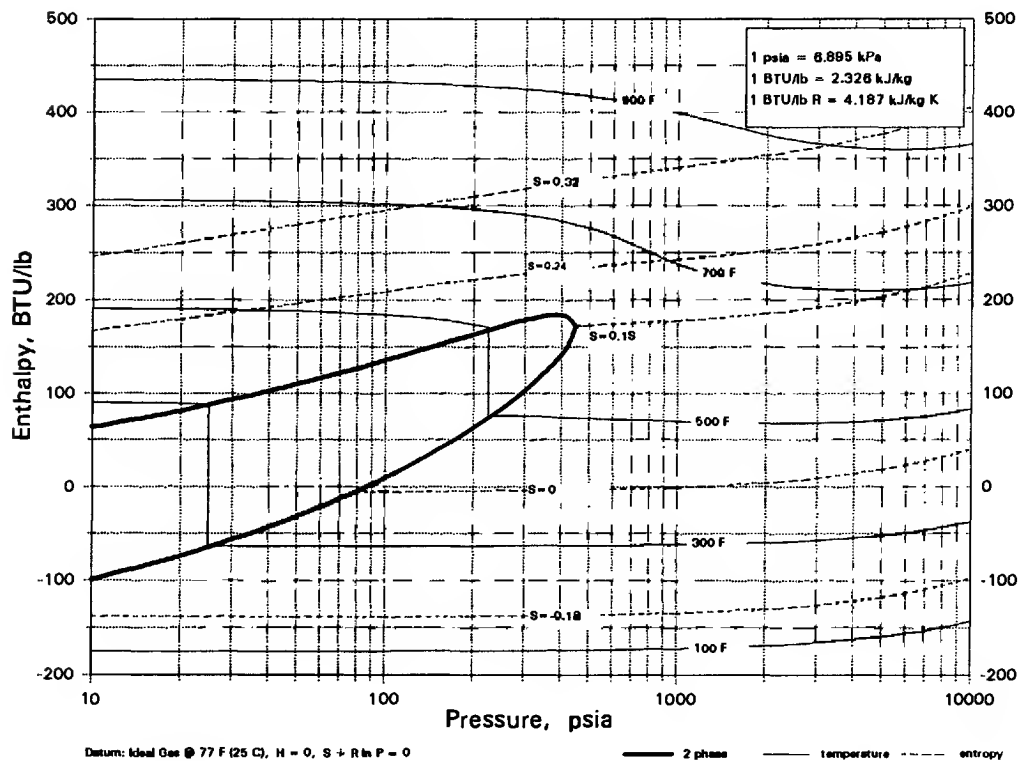
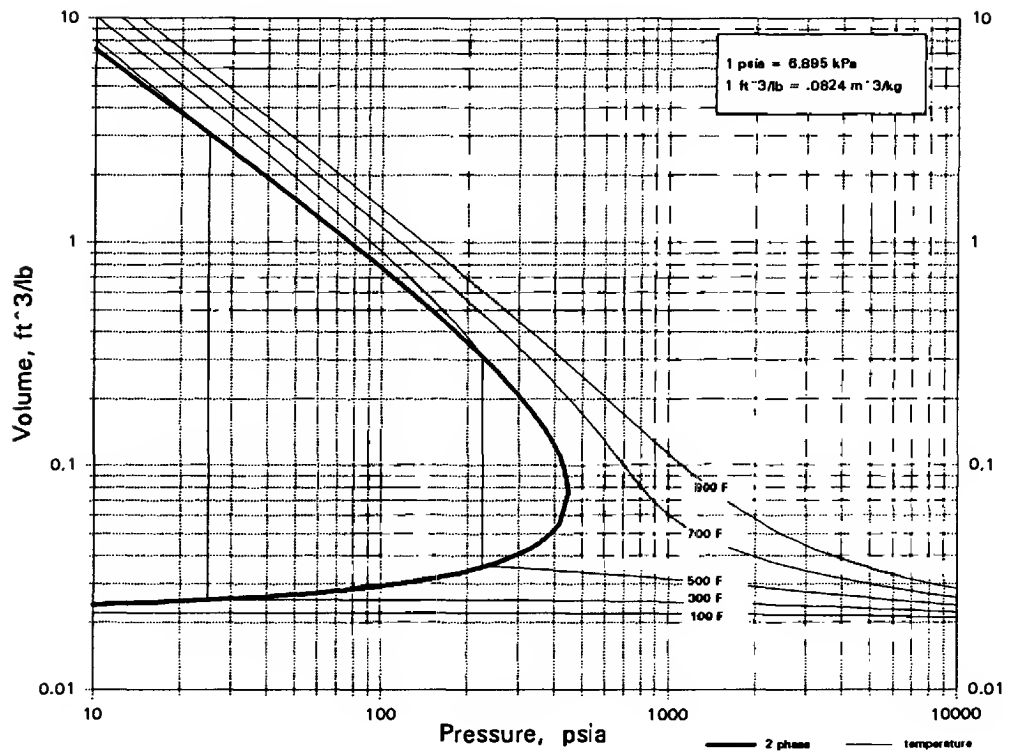


C6H12O

CYCLOHEXANOL

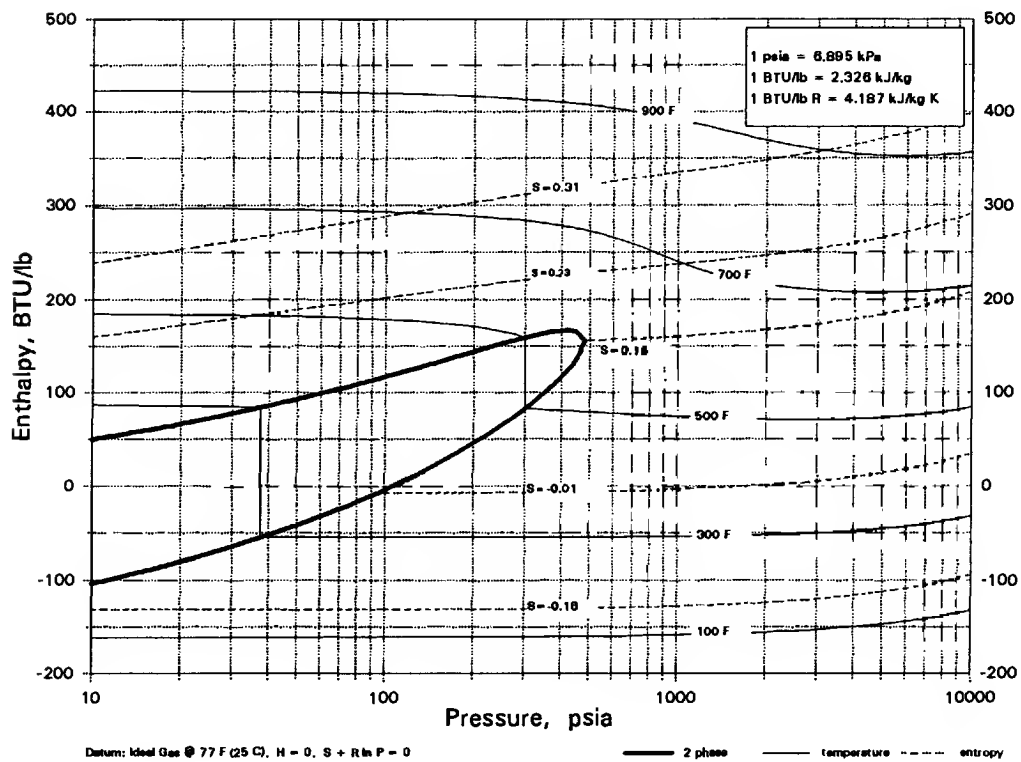
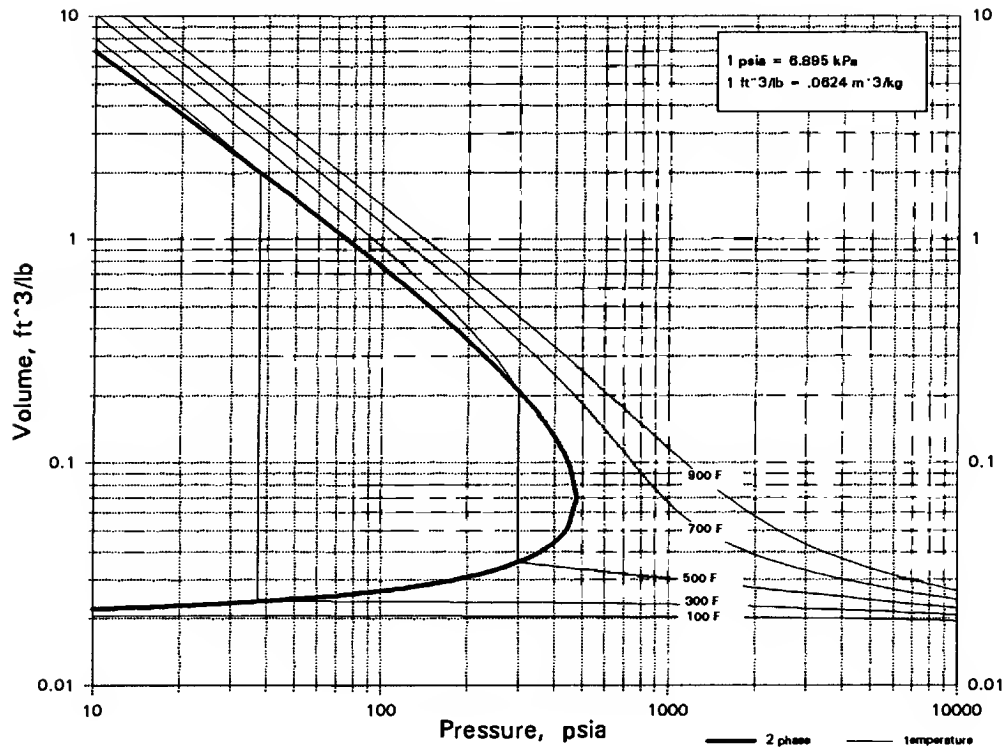


C6H12O
1-HEXANAL



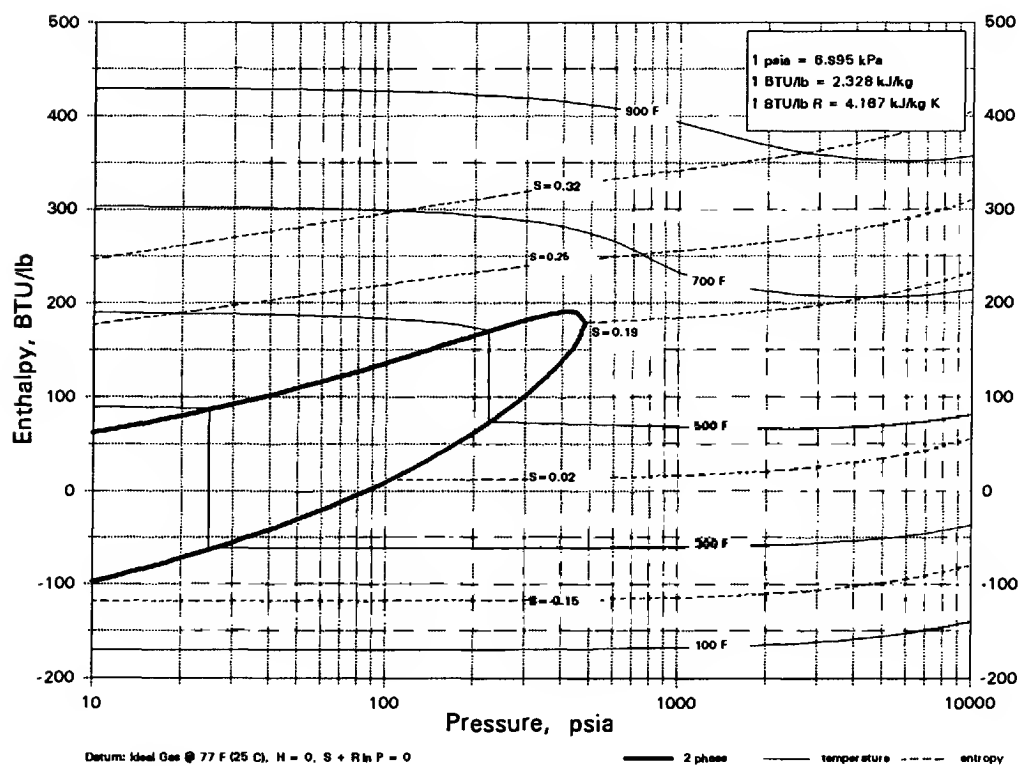
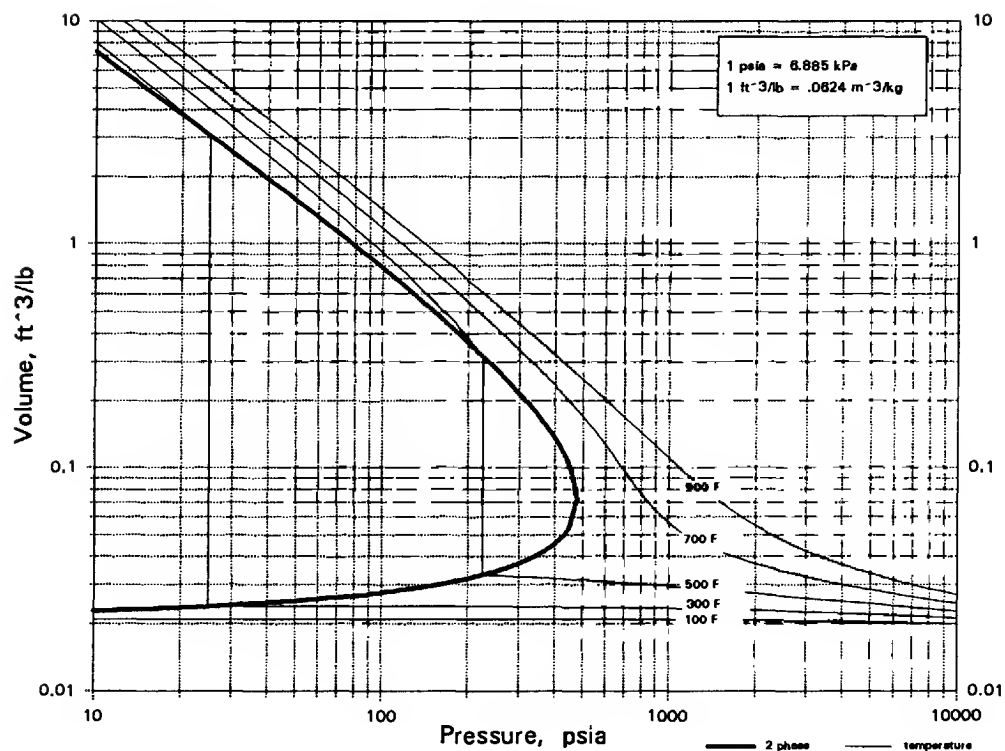
C6H12O

ETHYL ISOPROPYL KETONE



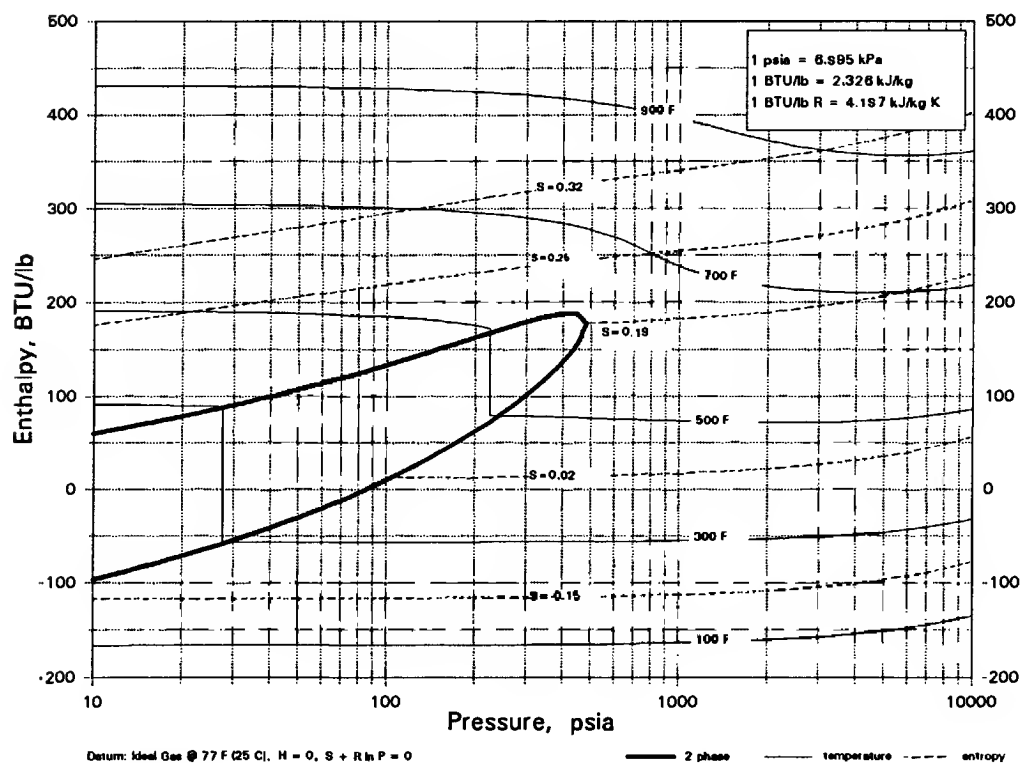
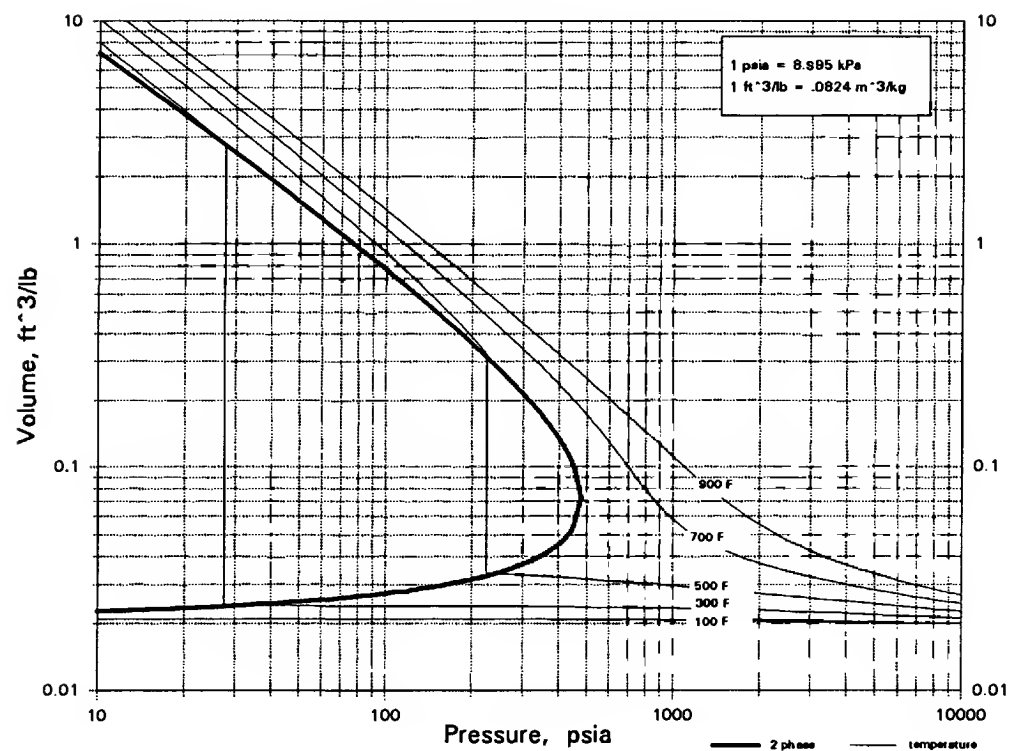
C6H12O

2-HEXANONE



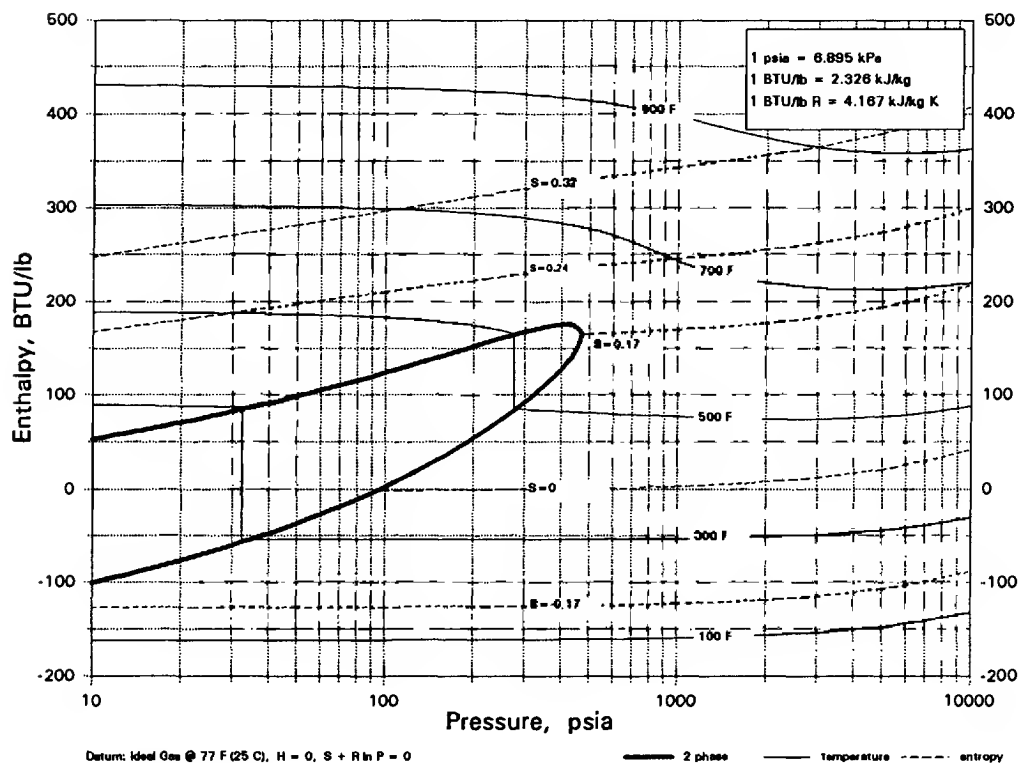
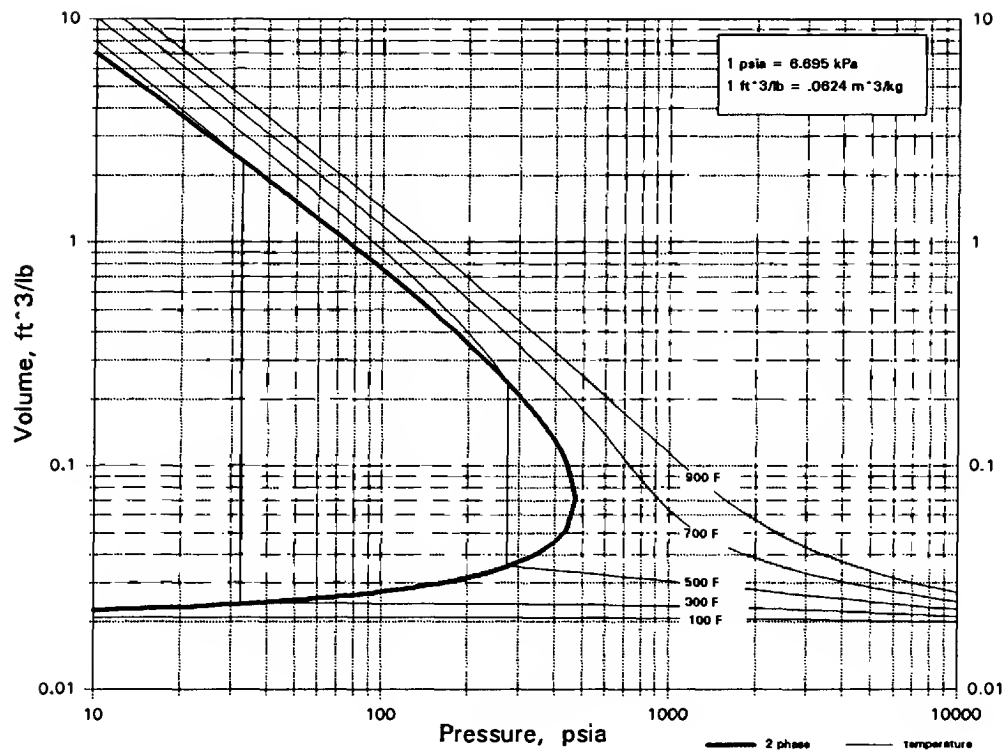
C6H12O

3-HEXANONE



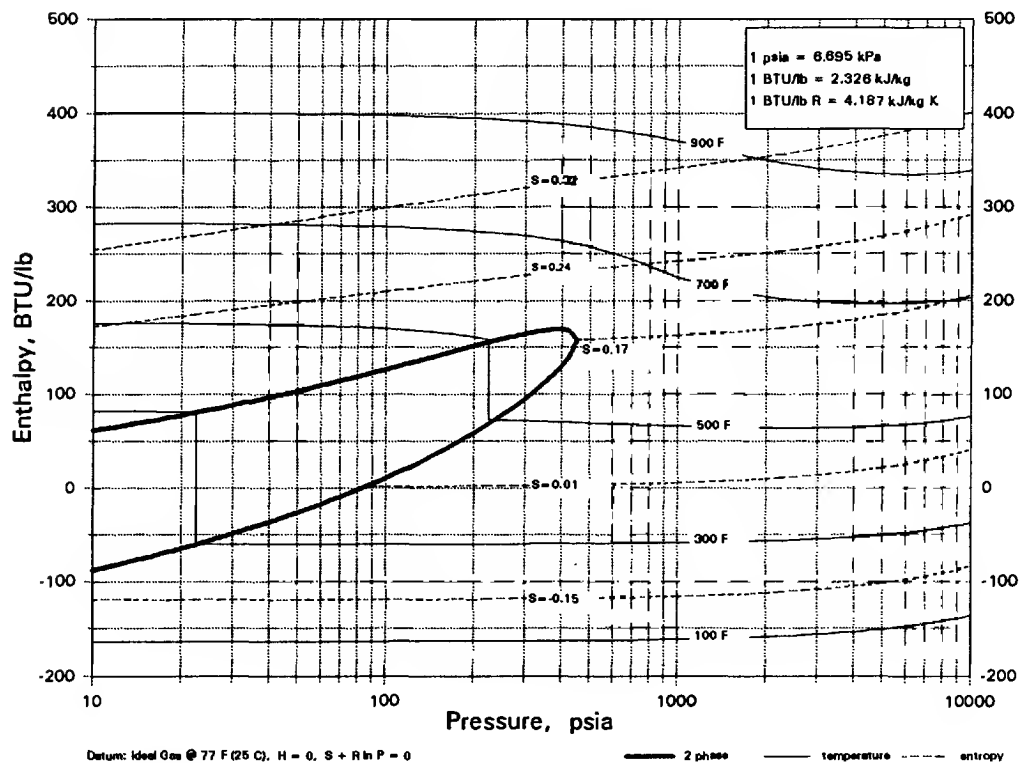
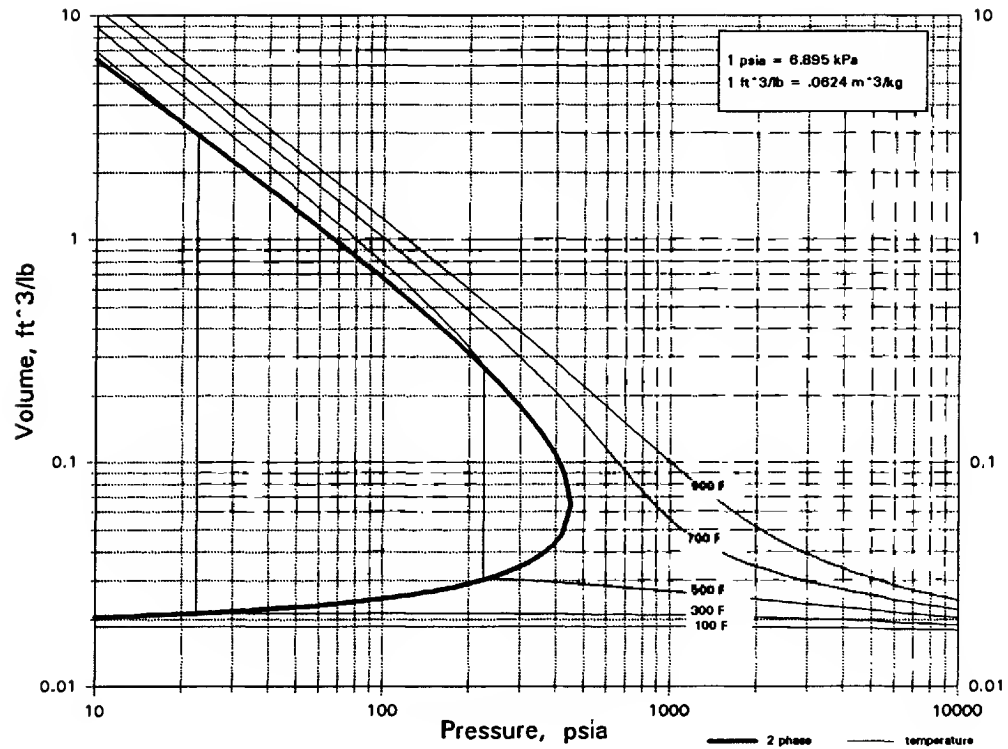
C6H12O

METHYL ISOBUTYL KETONE



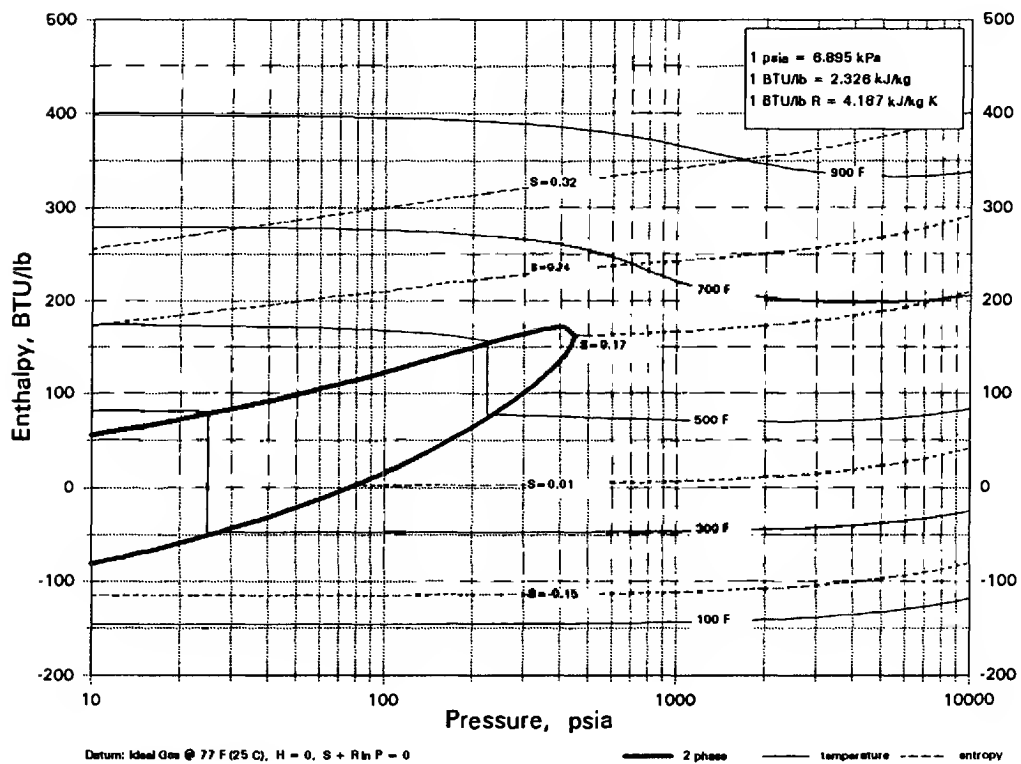
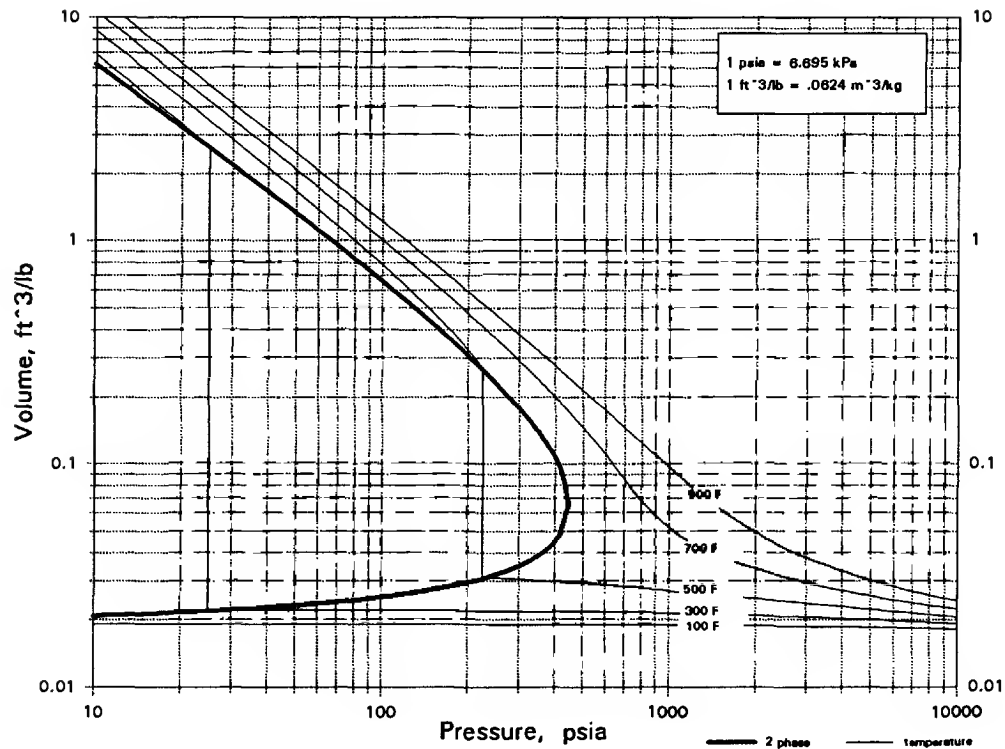
C6H12O2

n-PENTYL FORMATE



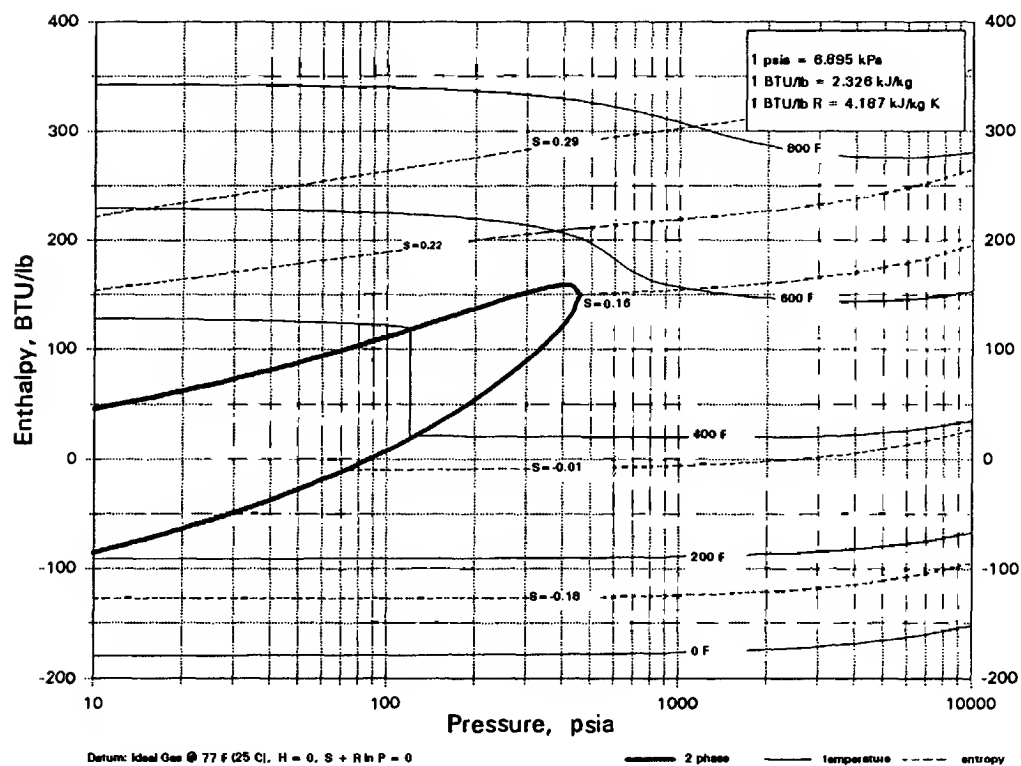
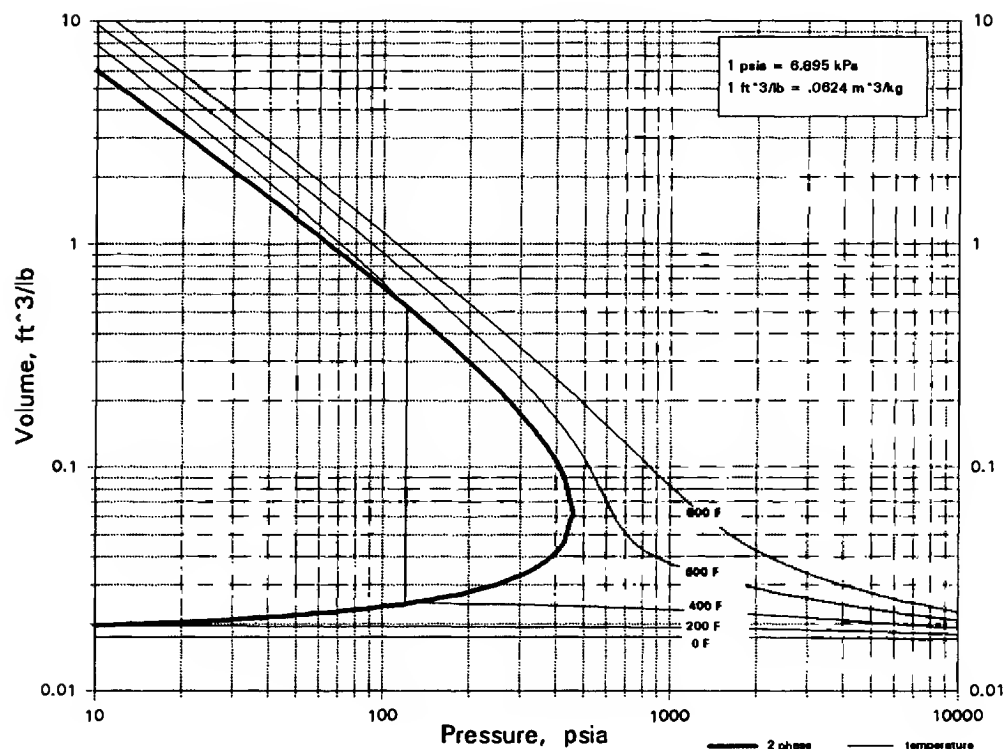
C6H12O2

n-BUTYL ACETATE



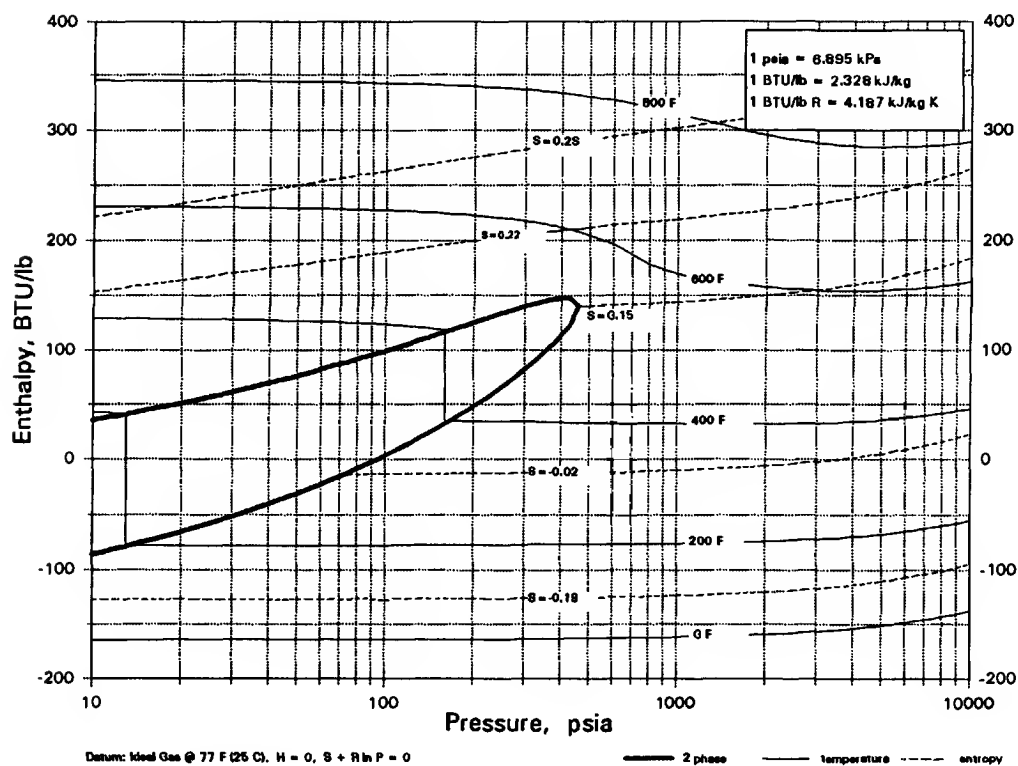
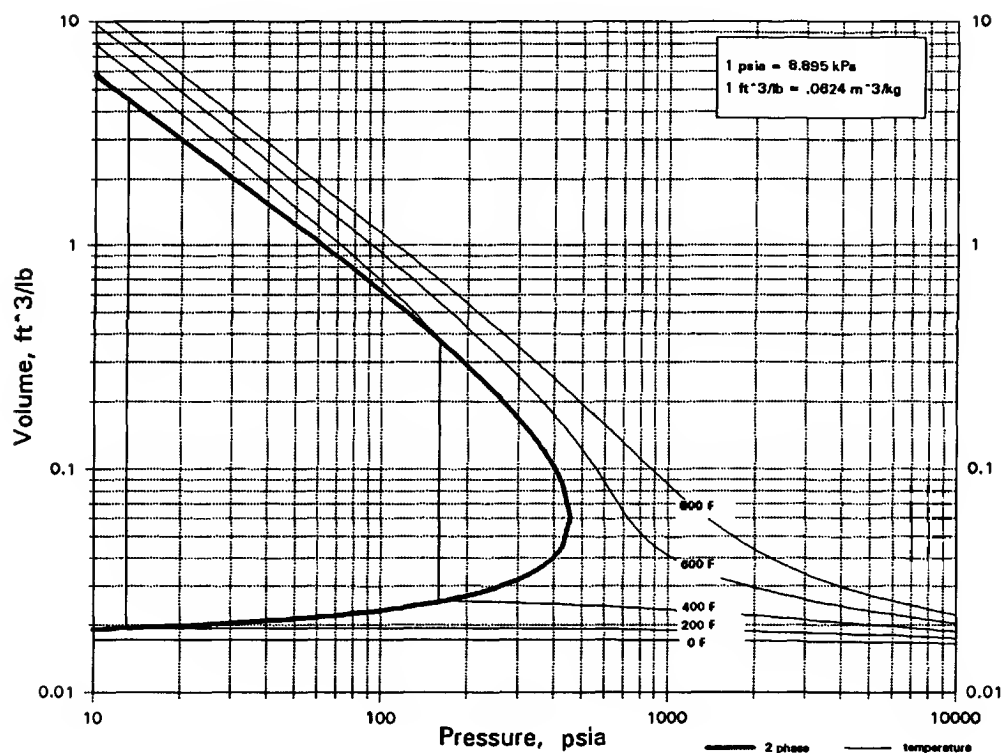
C6H12O2

sec-BUTYL ACETATE



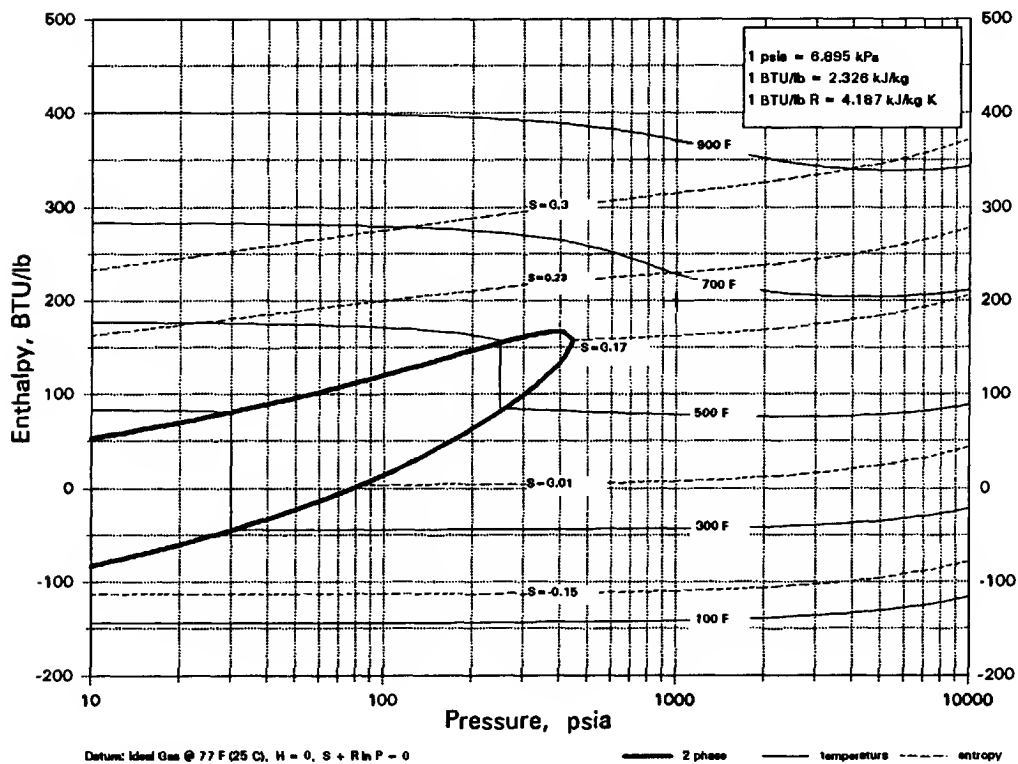
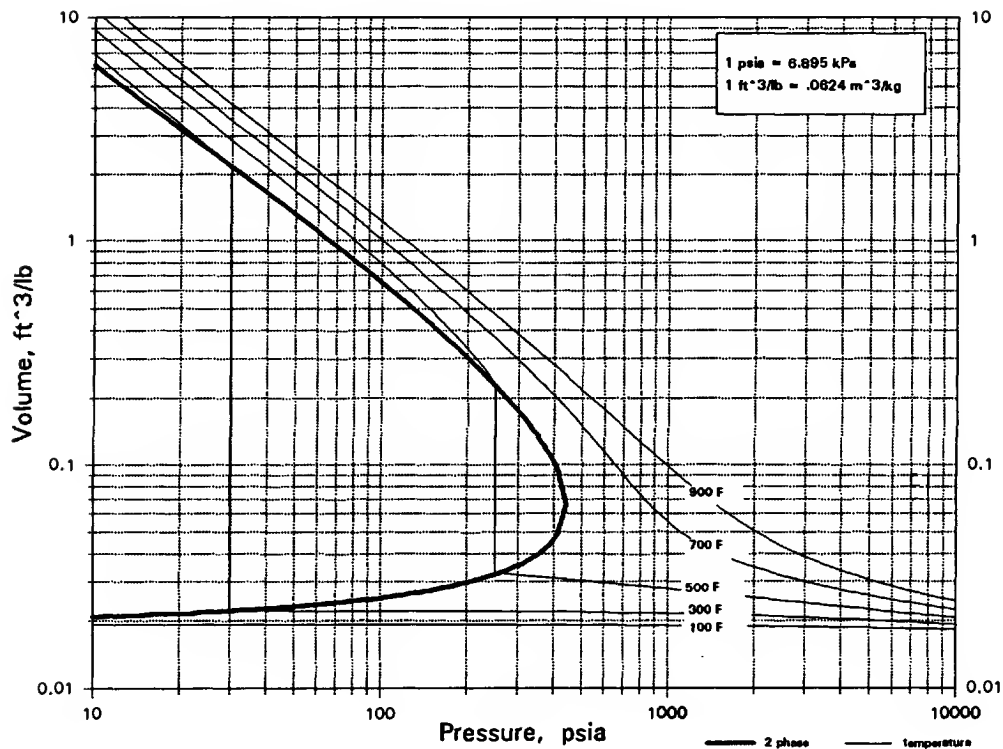
C6H12O2

tert-BUTYL ACETATE



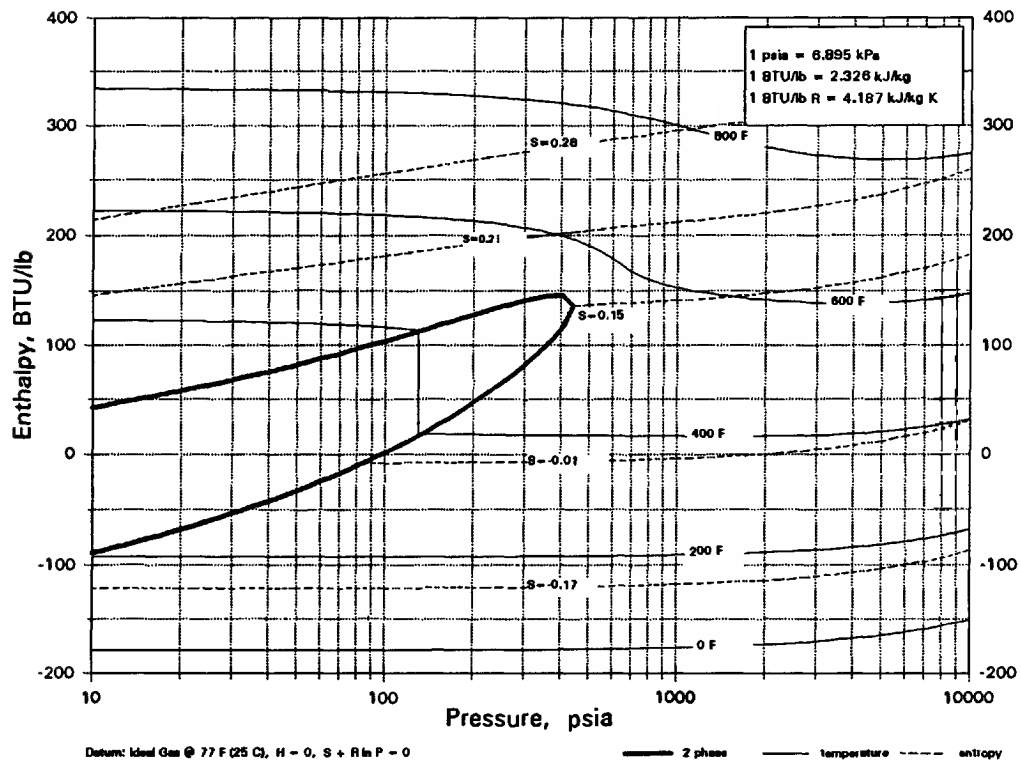
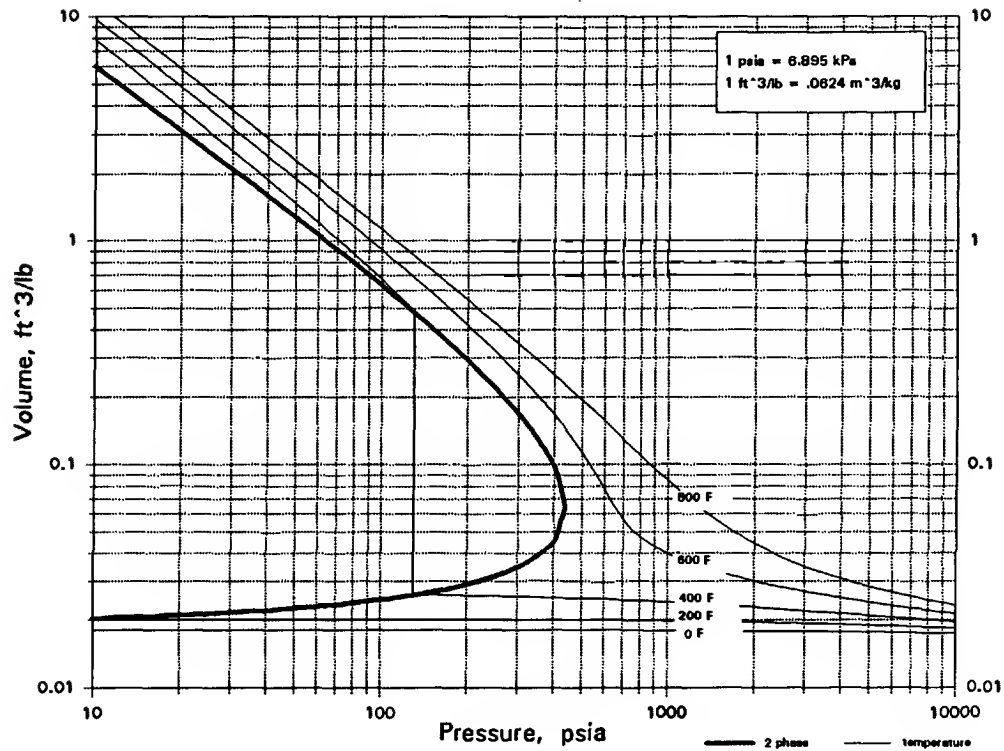
Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

C6H12O2
ETHYL n-BUTYRATE



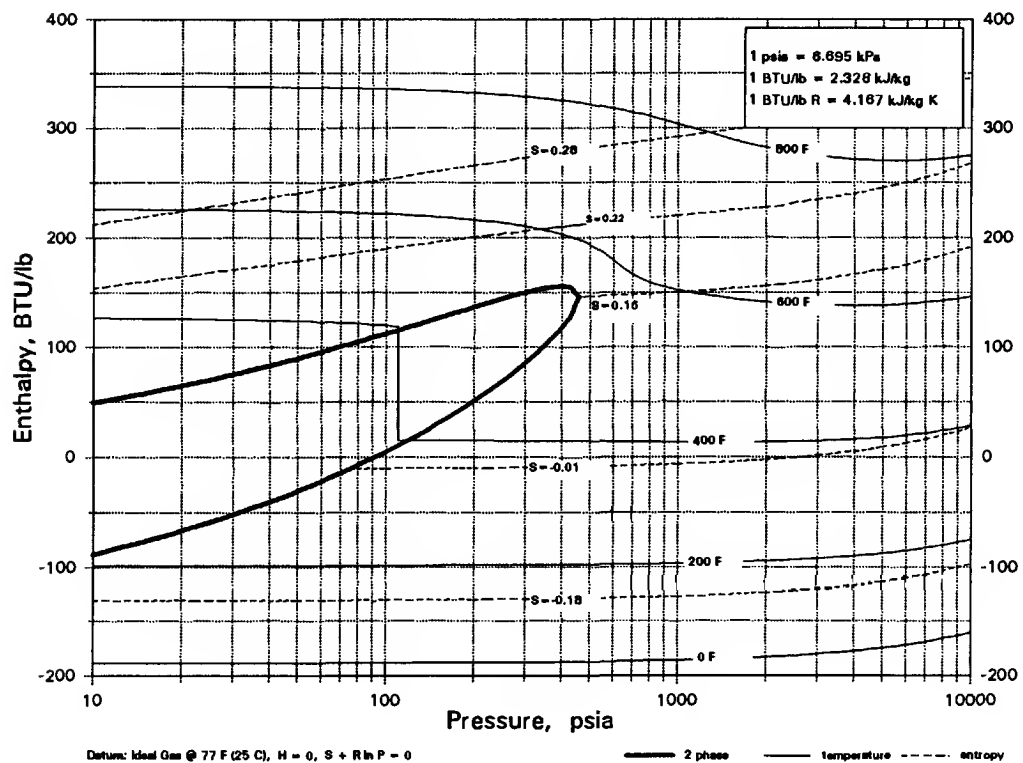
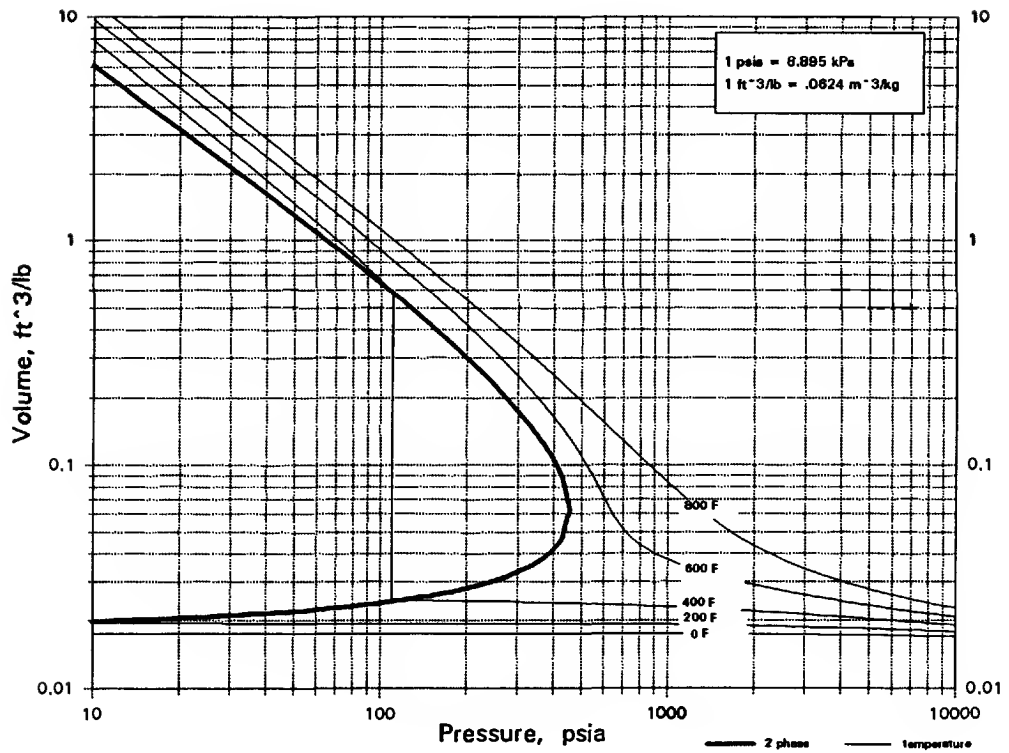
C6H12O2

ETHYL ISOBUTYRATE



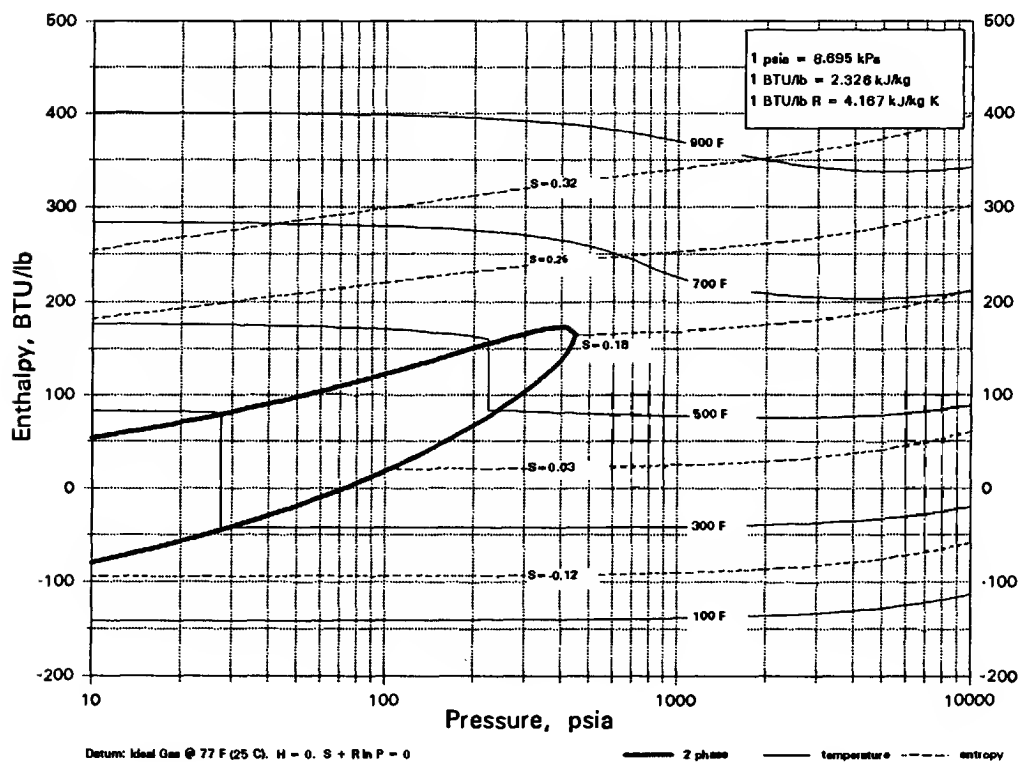
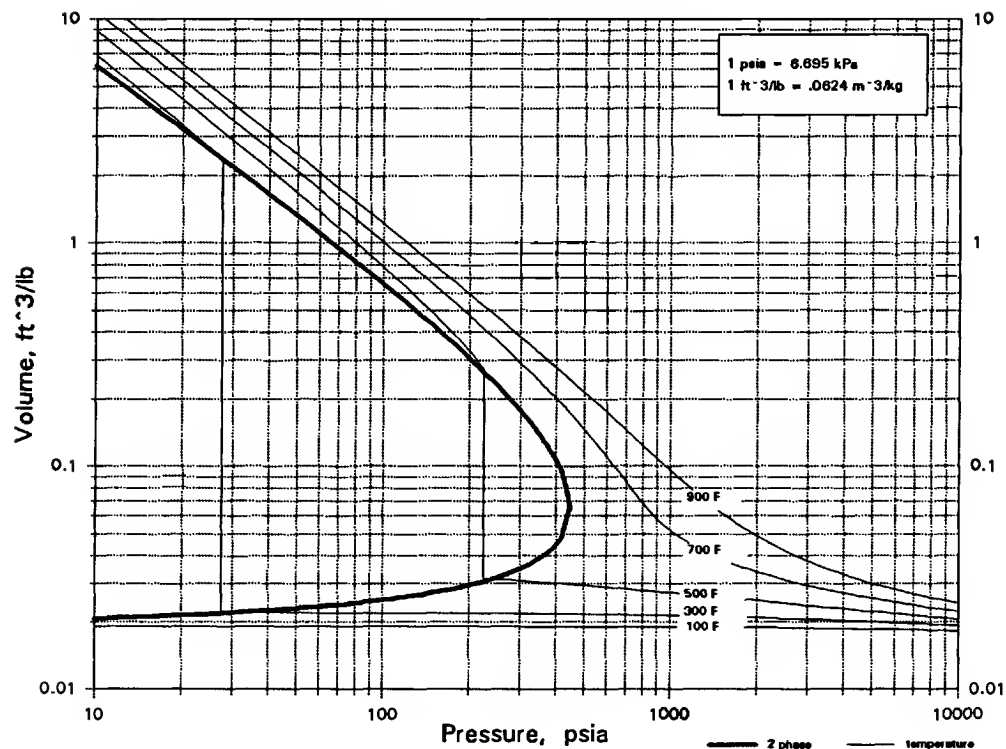
Deviation: Ideal Gas @ 77 F (25 C), H = 0, S = R ln P = 0

C6H12O2
ISOBUTYL ACETATE



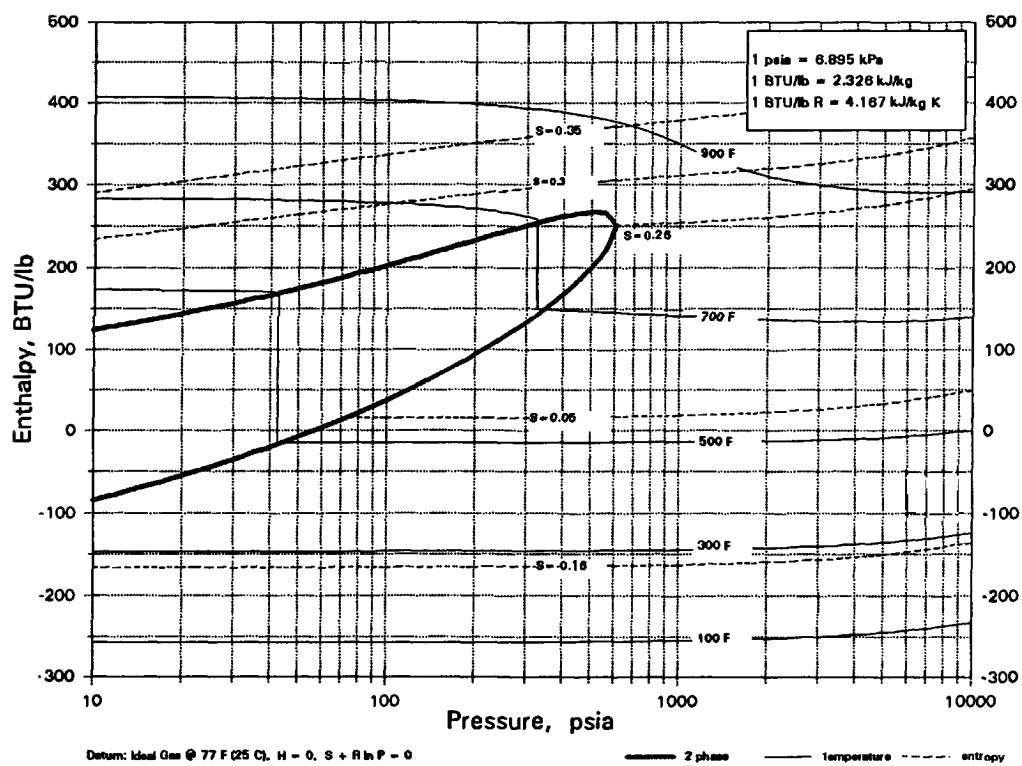
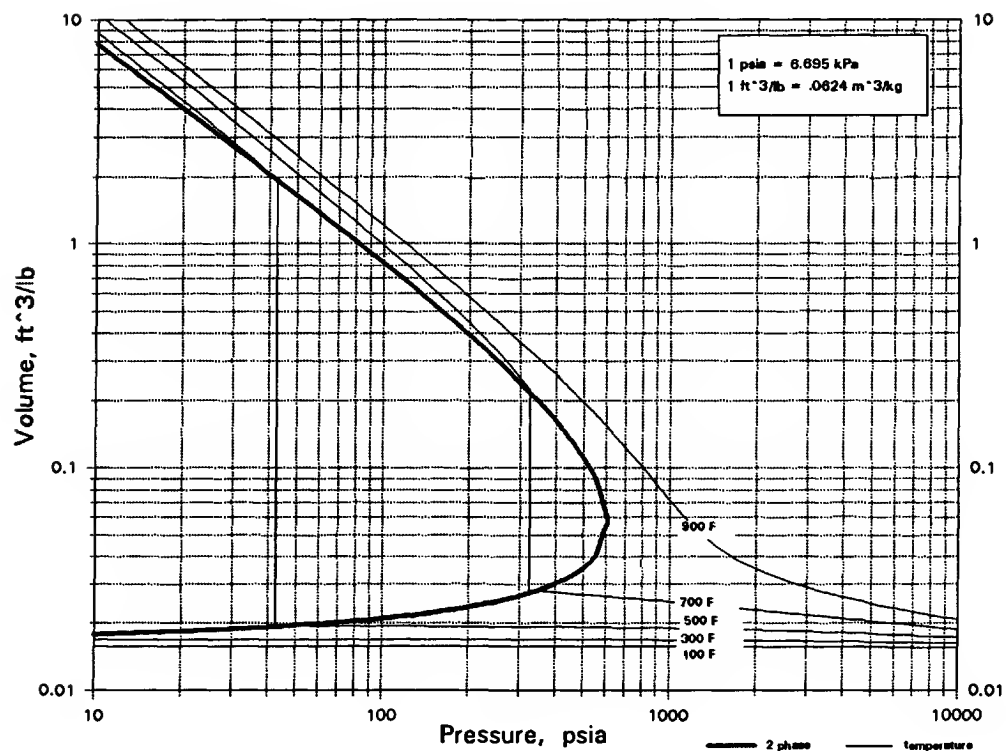
C6H12O2

n-PROPYL PROPIONATE



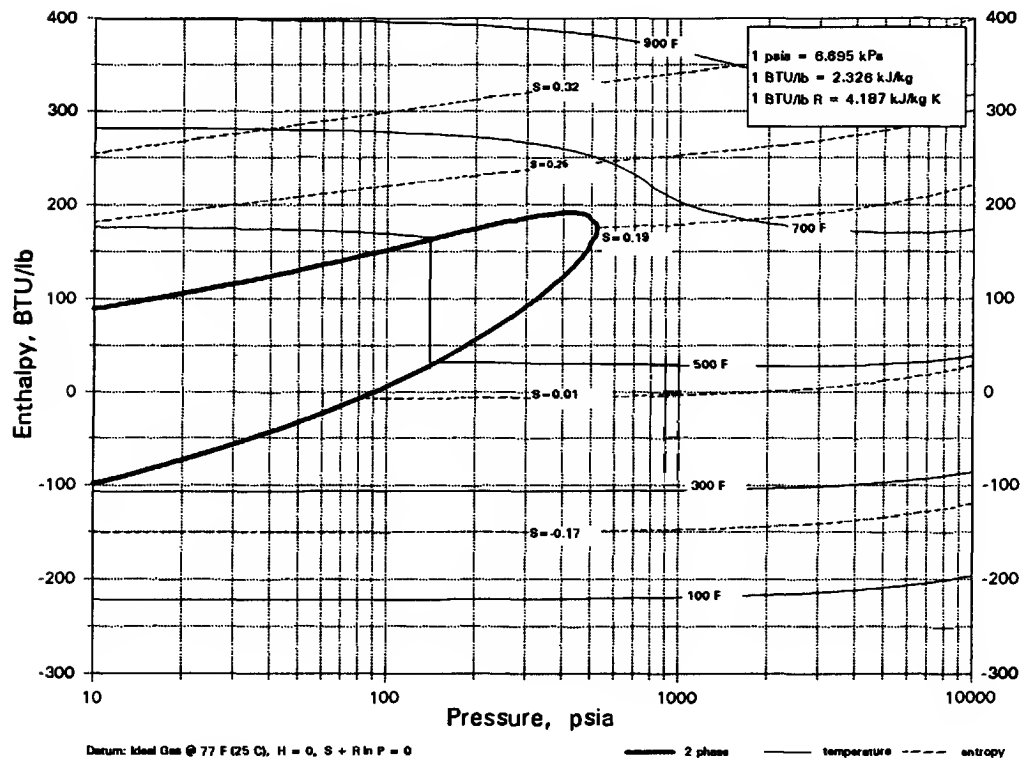
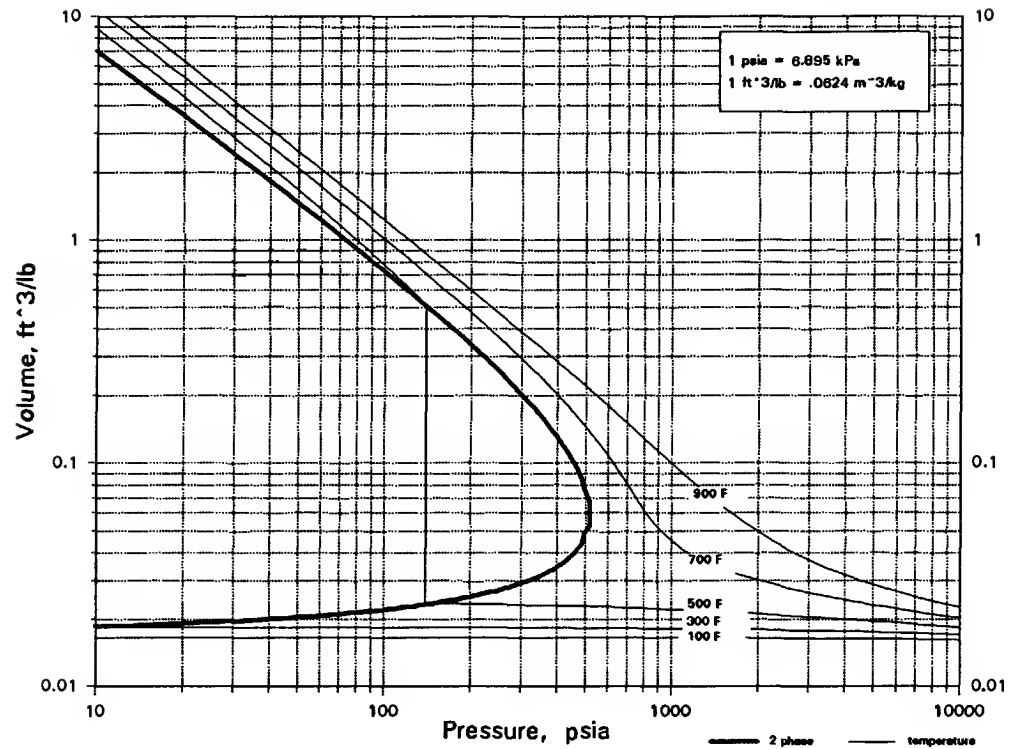
C6H12O2

CYCLOHEXYL PEROXIDE



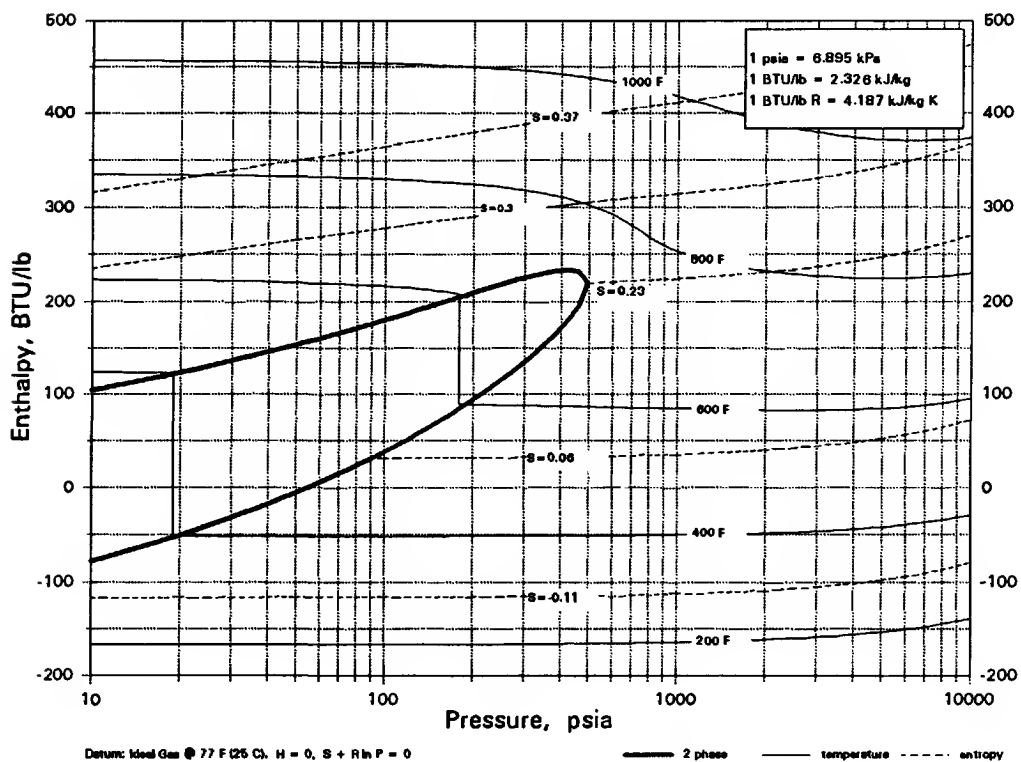
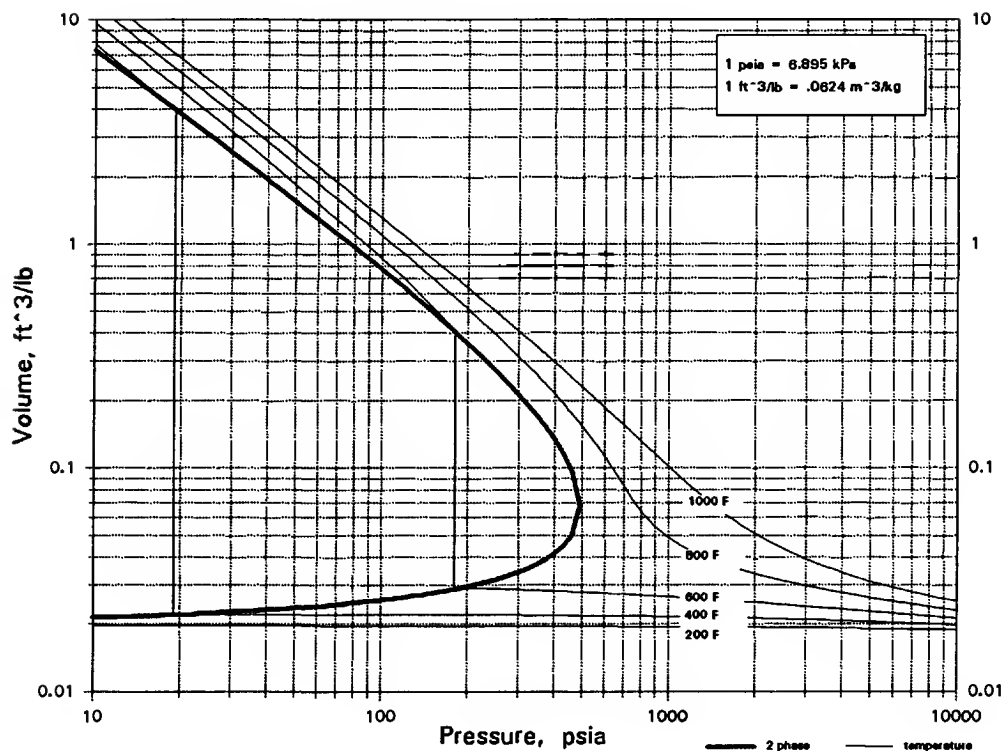
C6H12O2

DIACETONE ALCOHOL



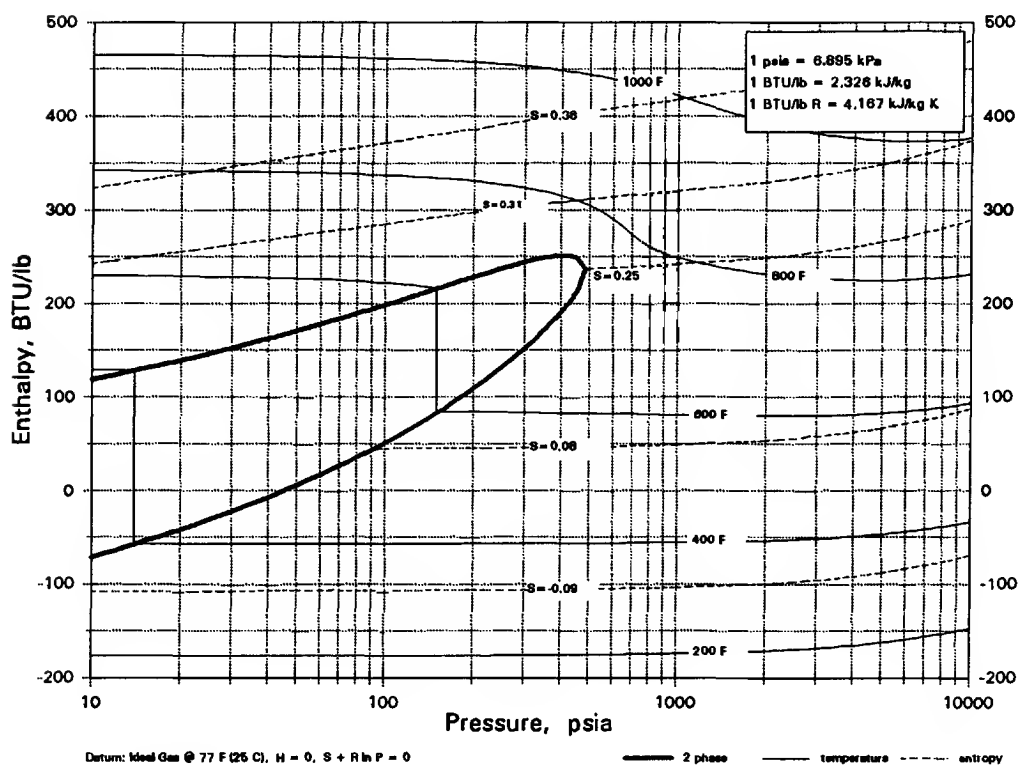
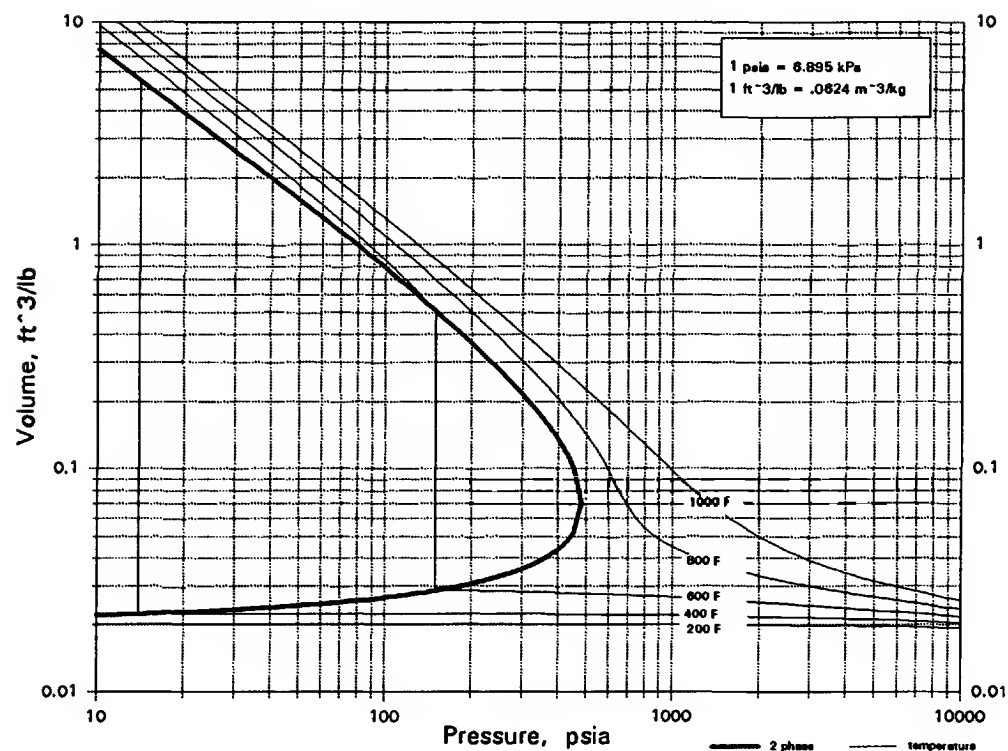
C6H12O2

2-ETHYL BUTYRIC ACID



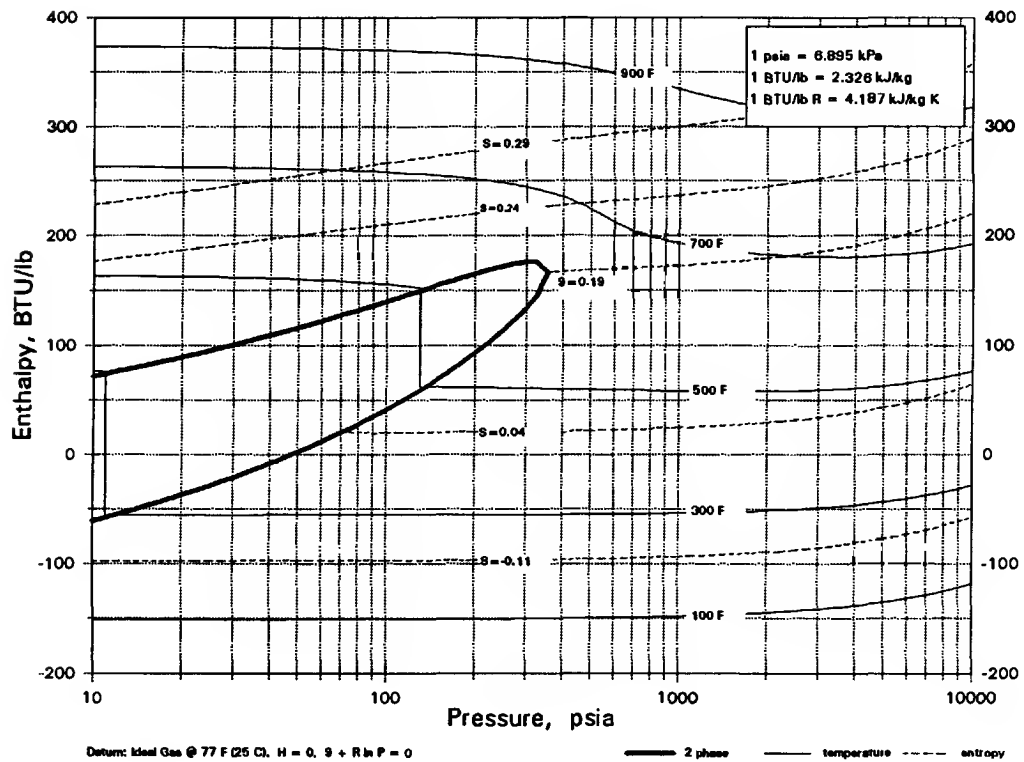
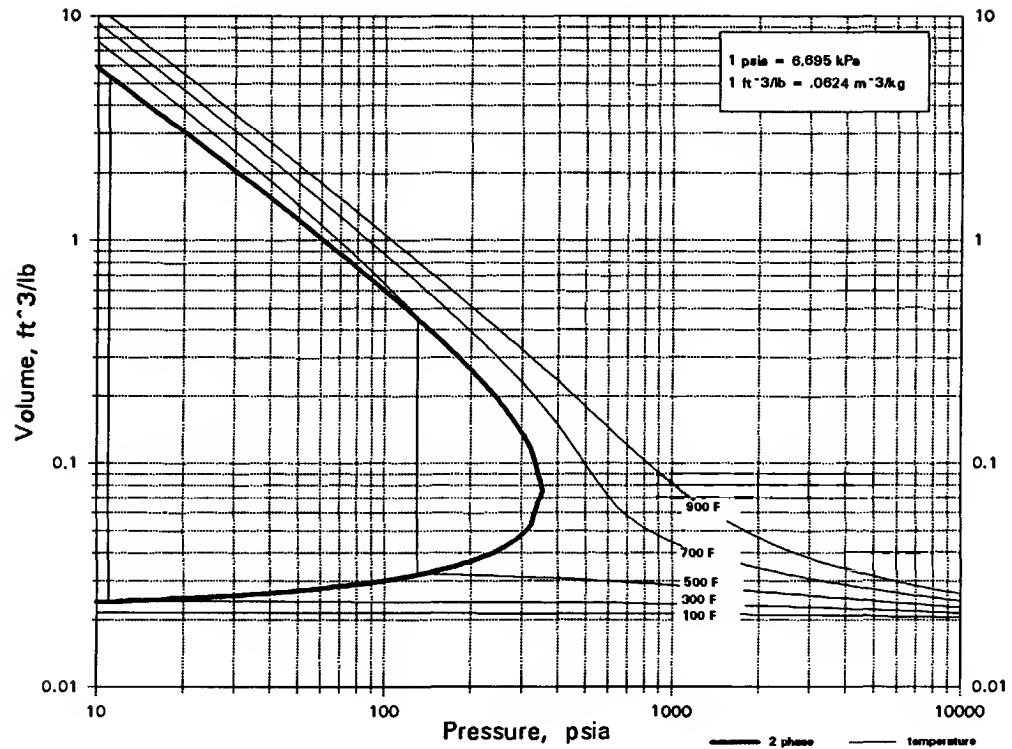
C6H12O2

n-HEXANOIC ACID



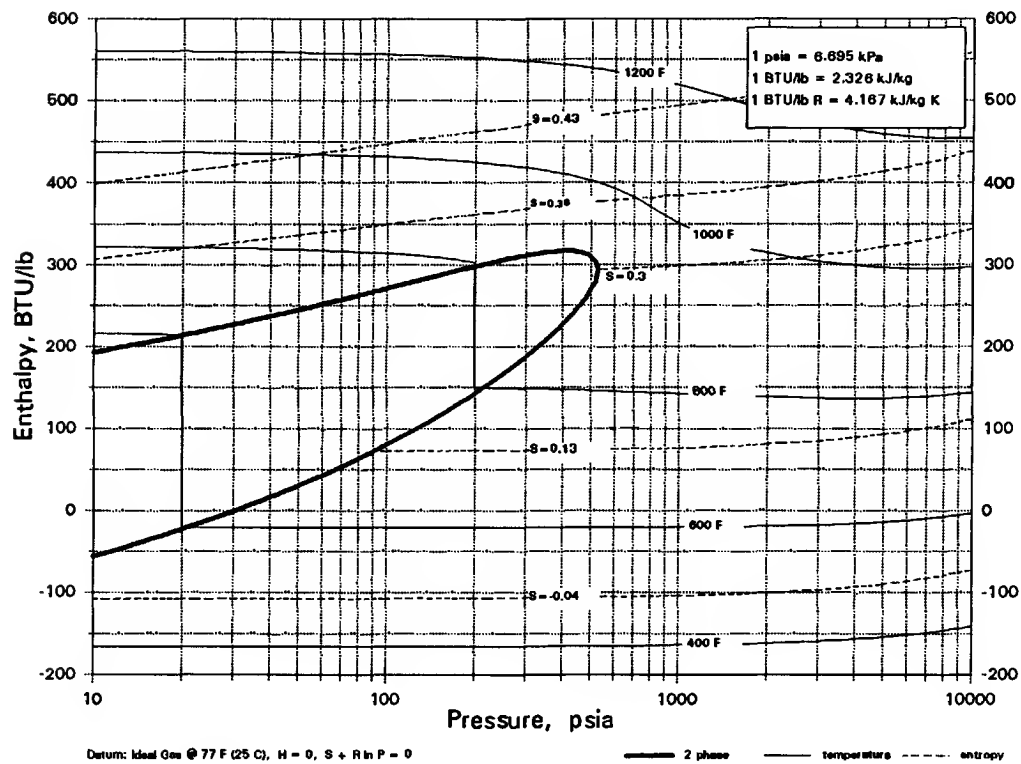
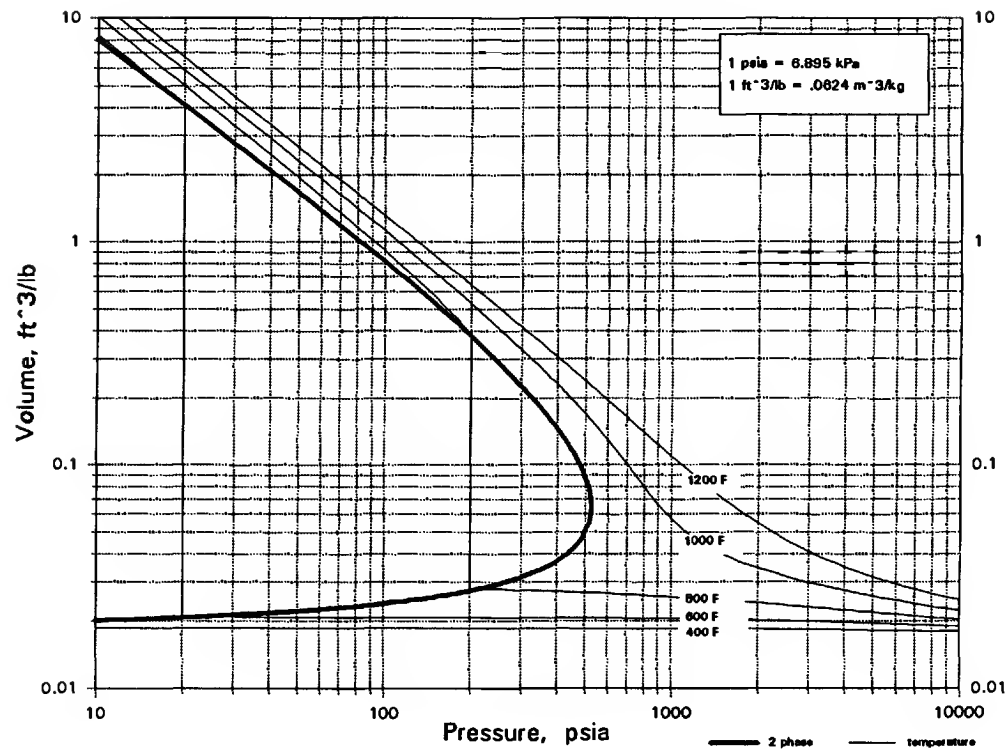
C6H12O3

2-ETHOXYETHYL ACETATE



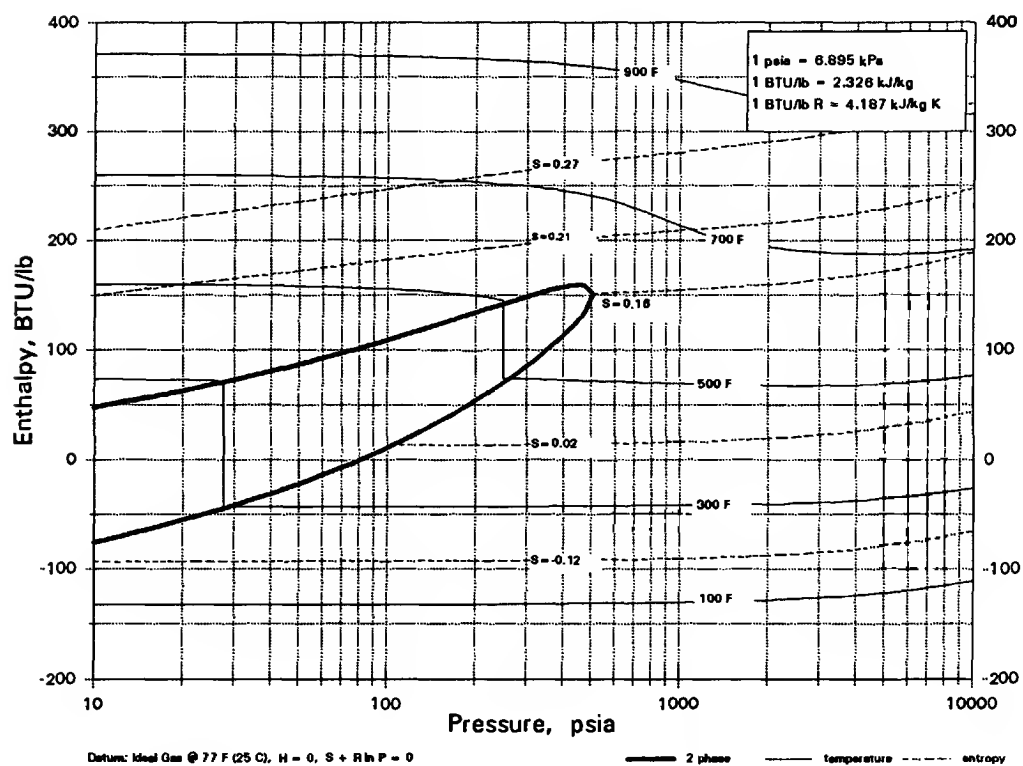
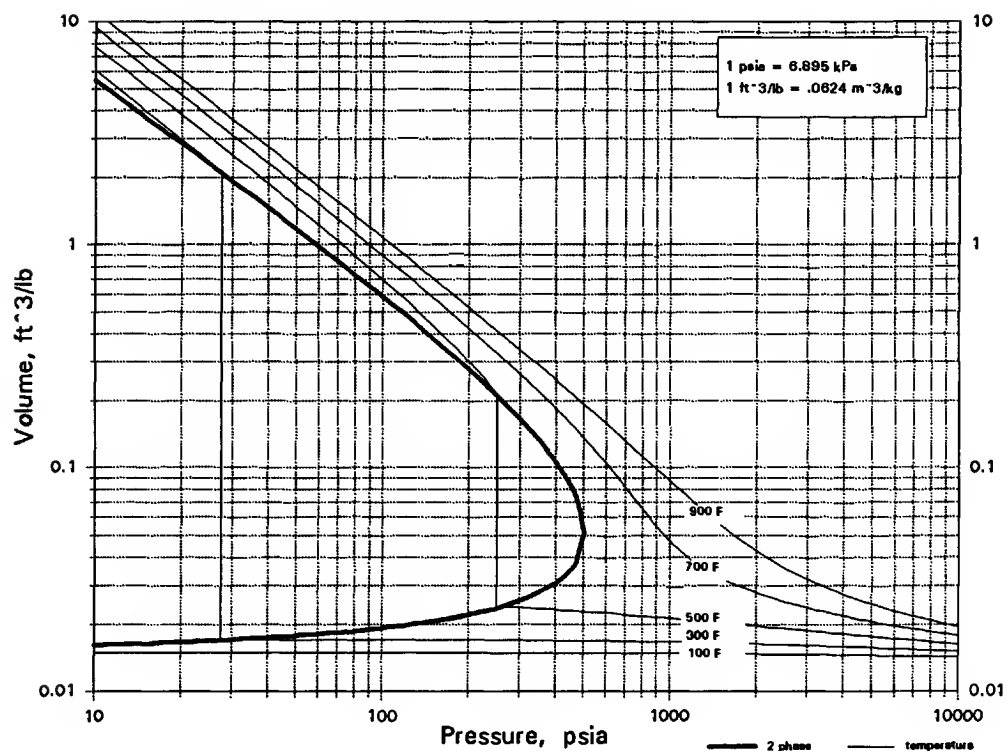
C6H12O3

HYDROXYCAPROIC ACID



C6H12O3

PARALDEHYDE



C6H12O3

sec-BUTYL GLYCOLATE

1. Molecular Weight, lb/mol..... 132.16

2. Boiling Point, K..... 450.65

Critical data (Tc, Pc) are not available.

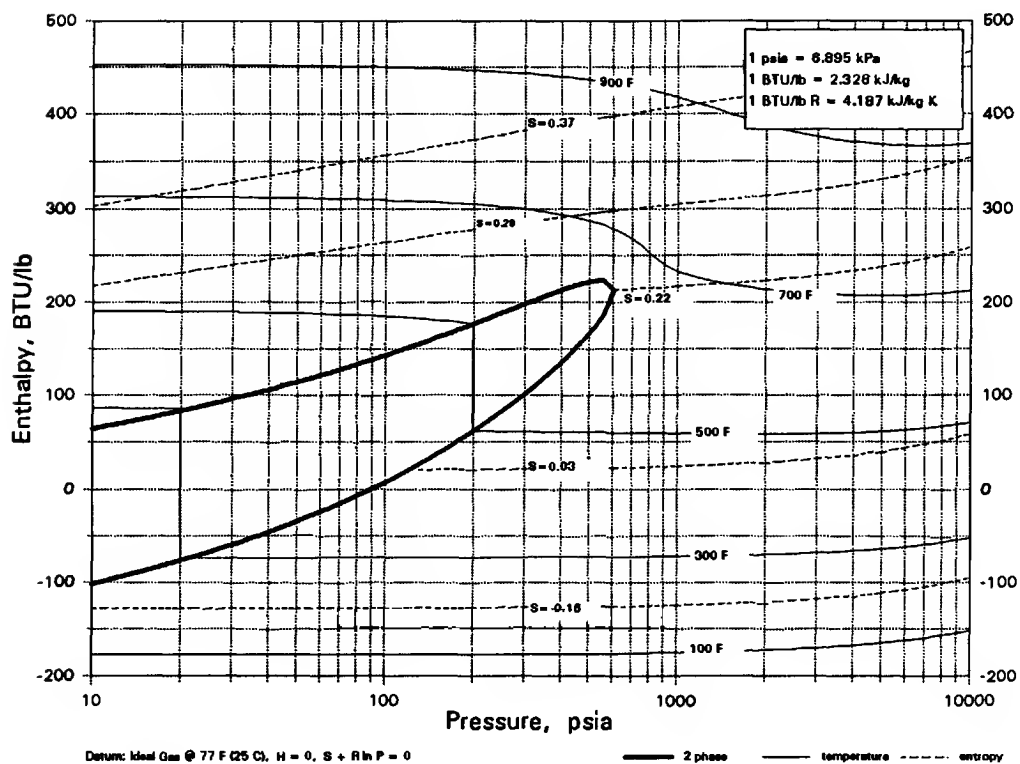
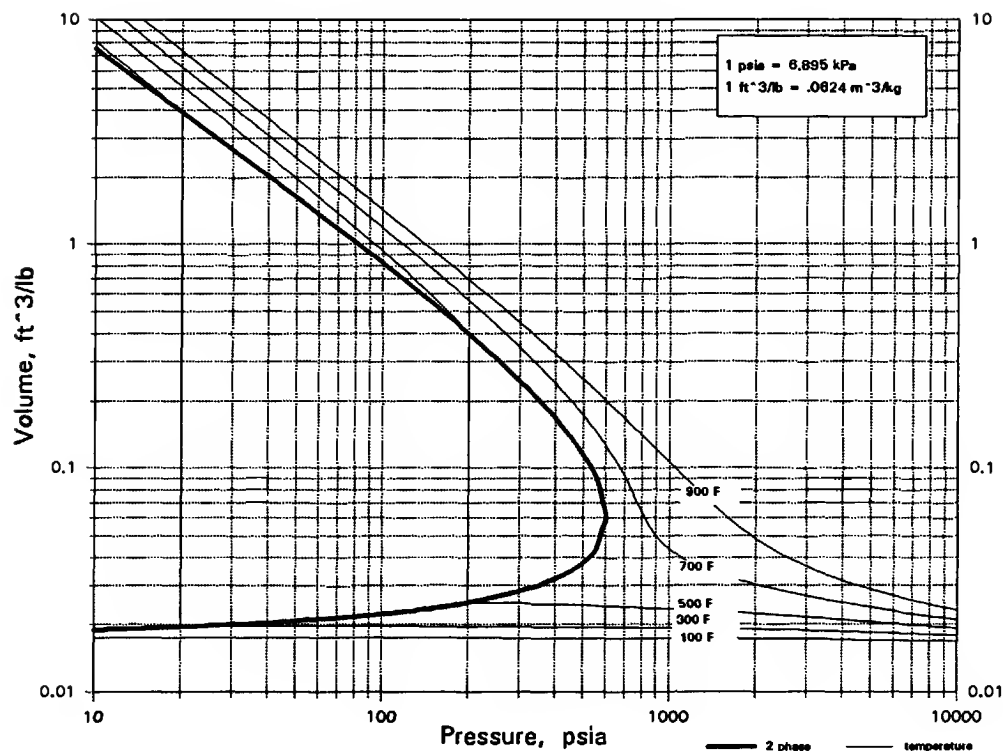
1. Molecular Weight, lb/mol..... 132.16

2. Boiling Point, K..... 450.65

Critical data (Tc, Pc) are not available.

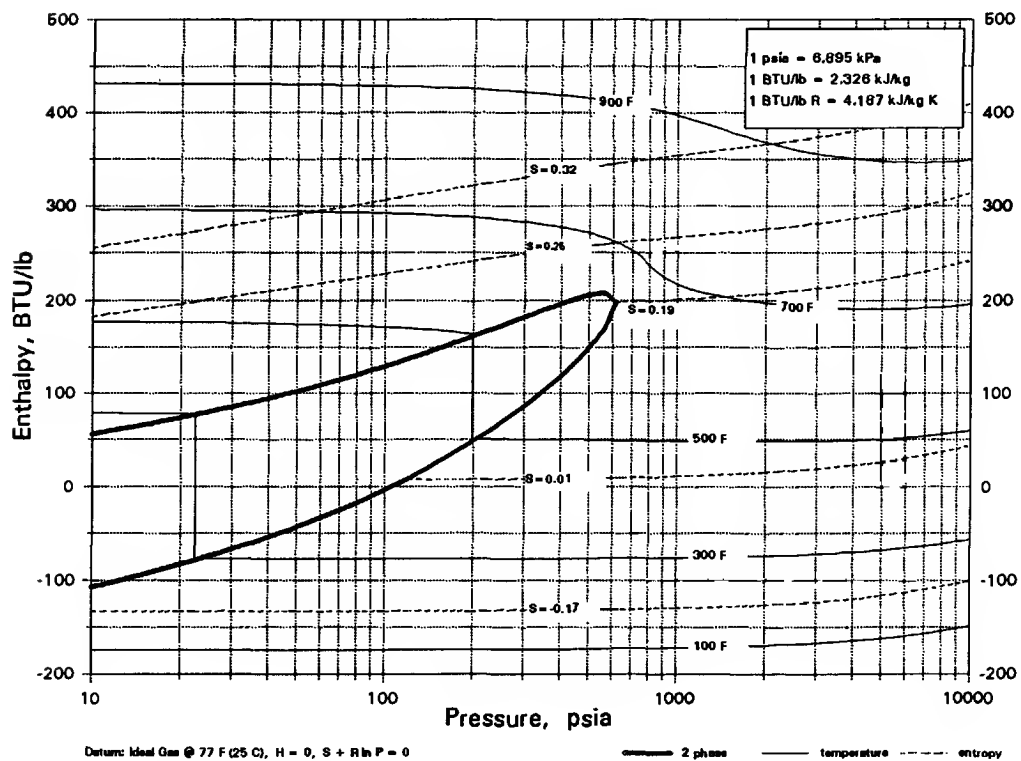
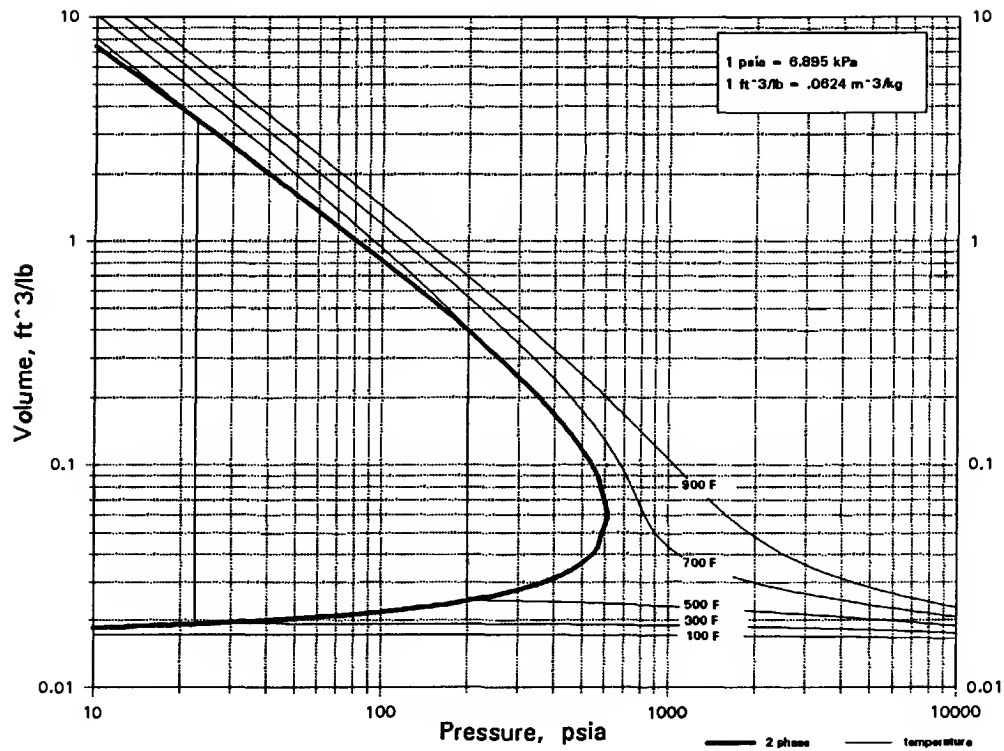
C6H13N

CYCLOHEXYLAMINE



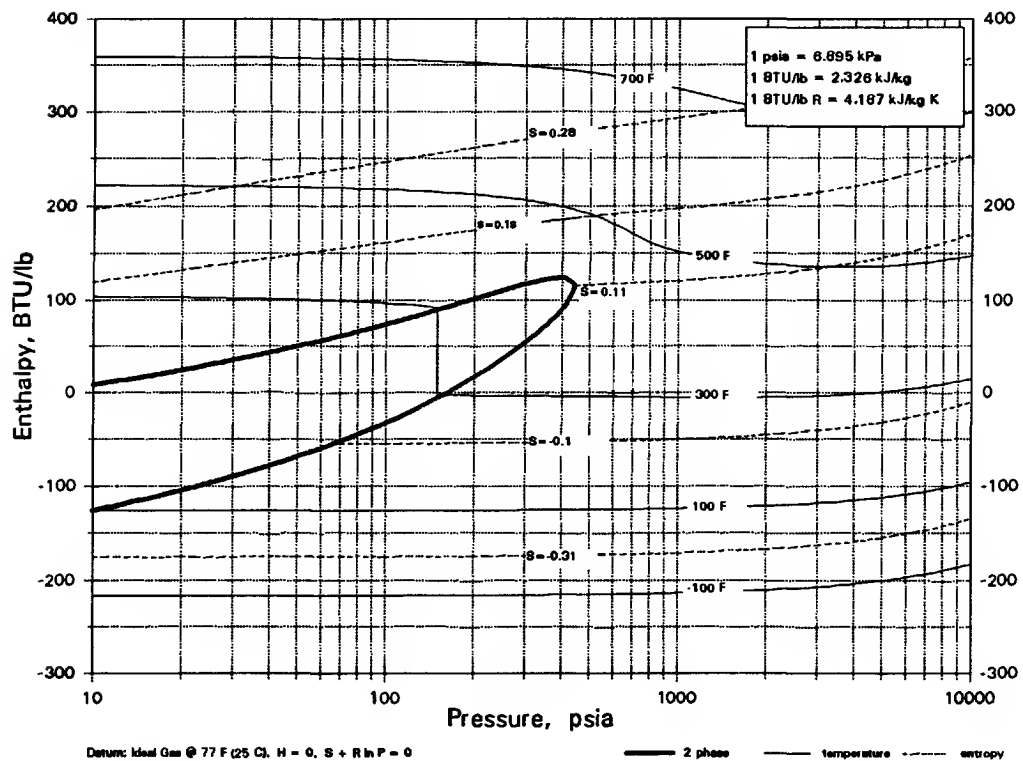
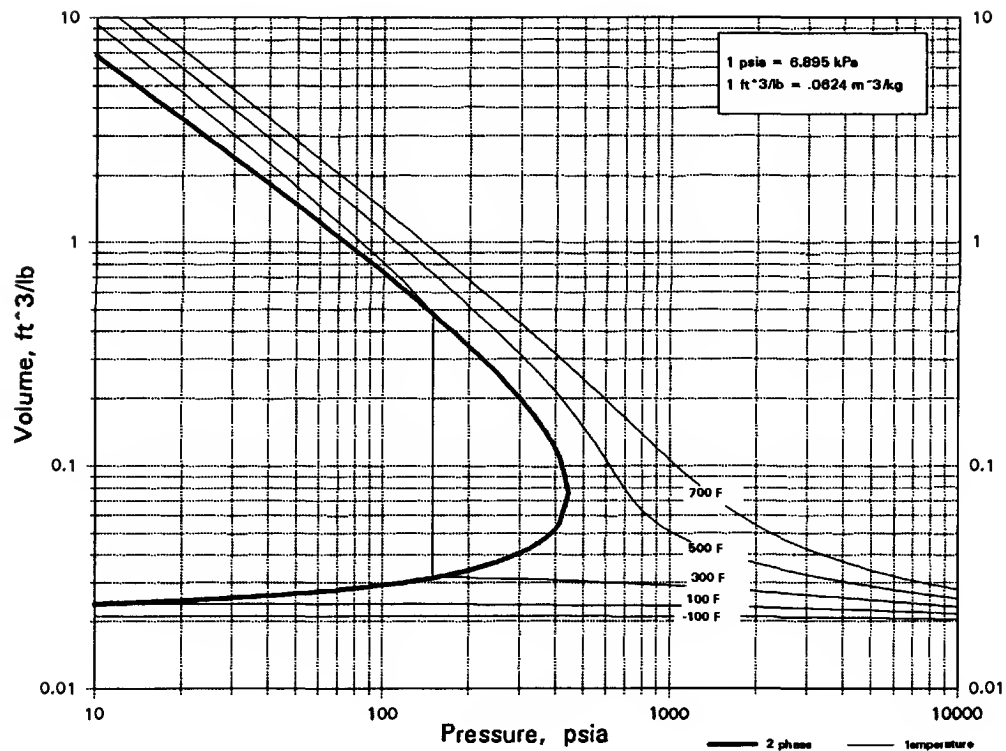
C6H13N

HEXAMETHYLENEIMINE



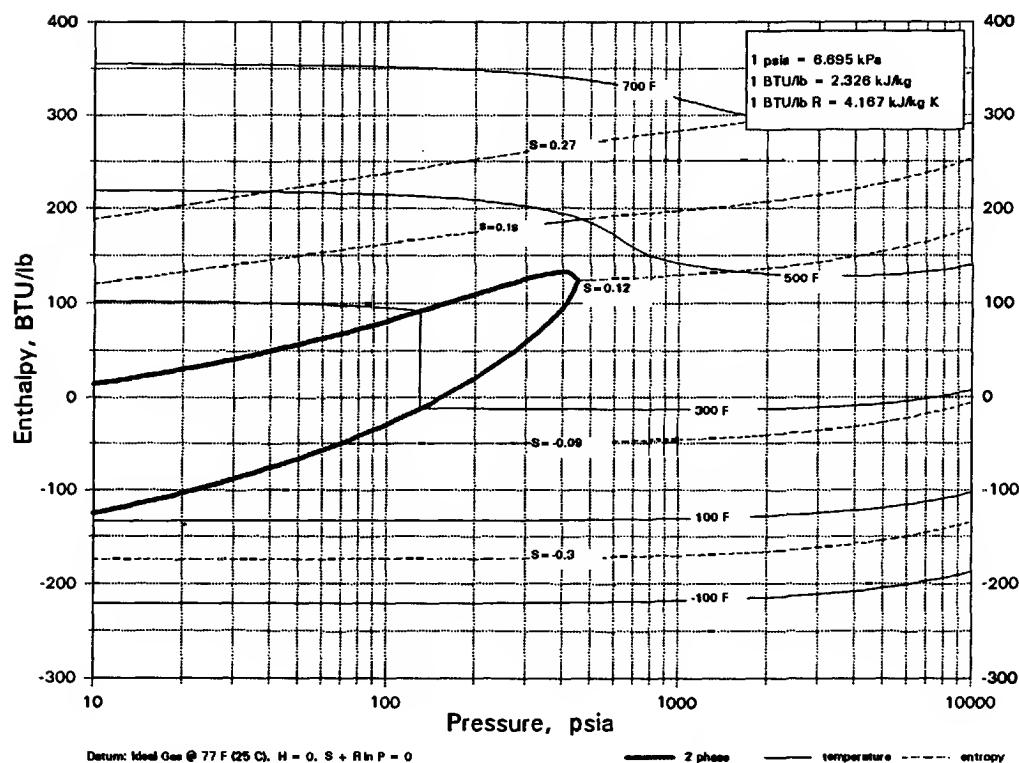
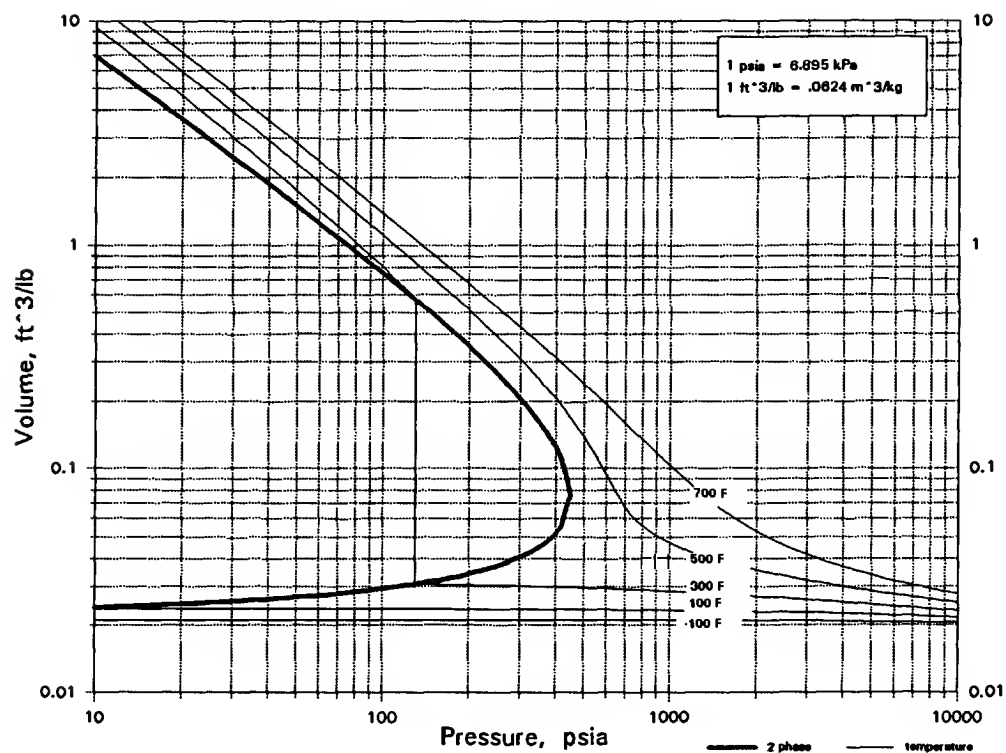
C6H14

2-2-DIMETHYLBUTANE



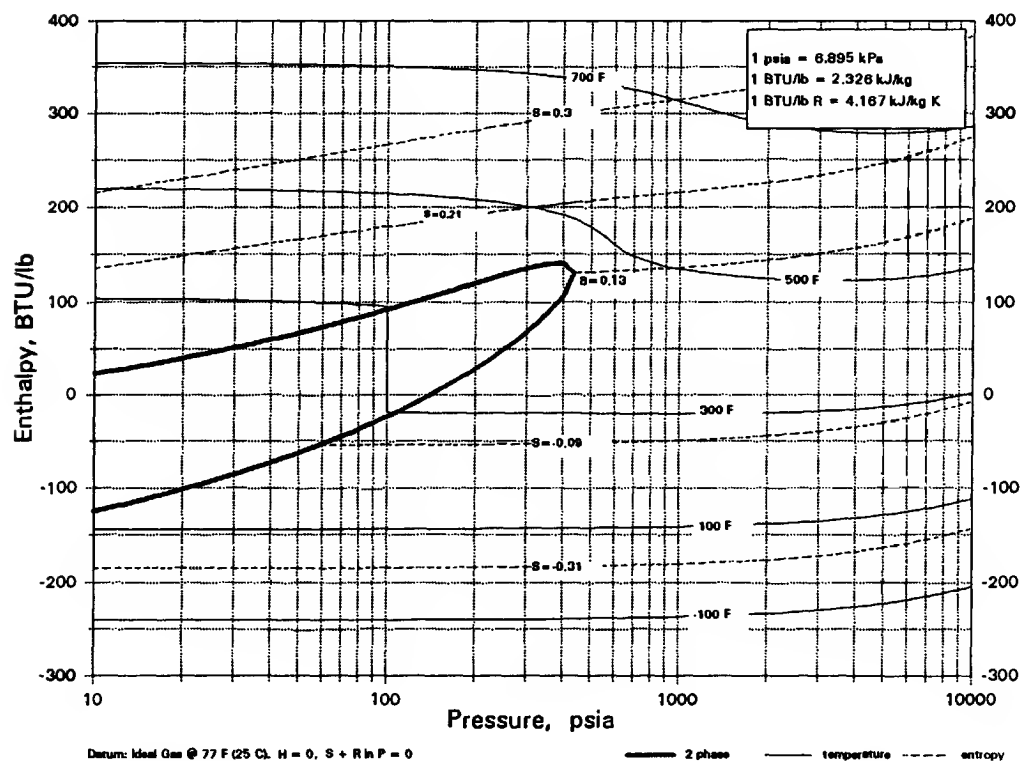
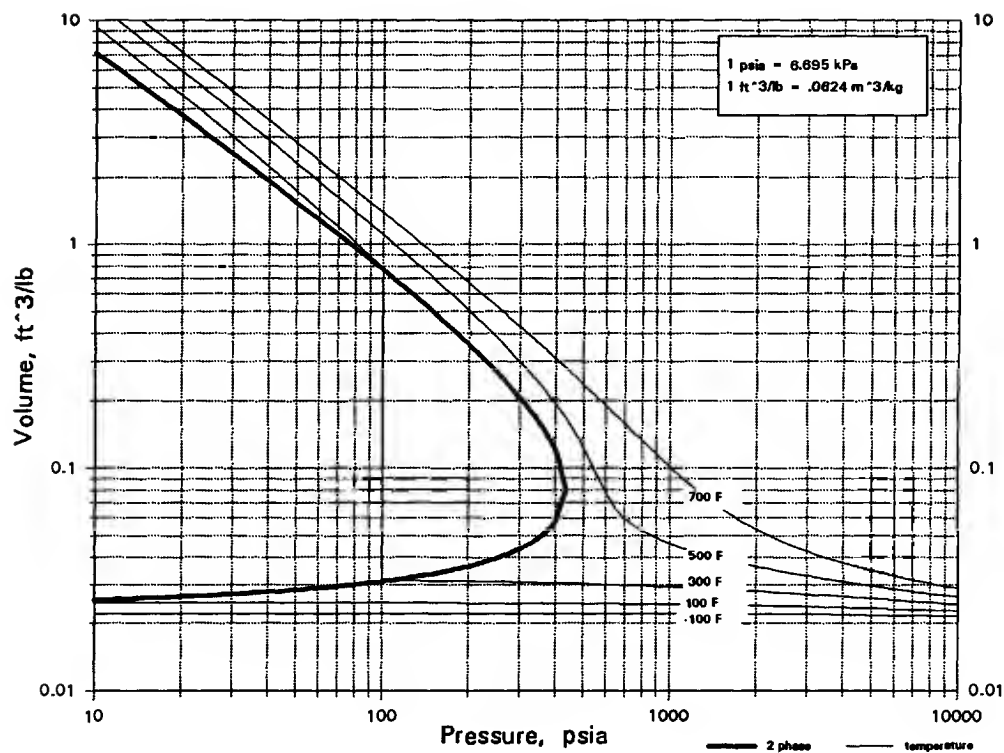
C6H14

2-3-DIMETHYLBUTANE

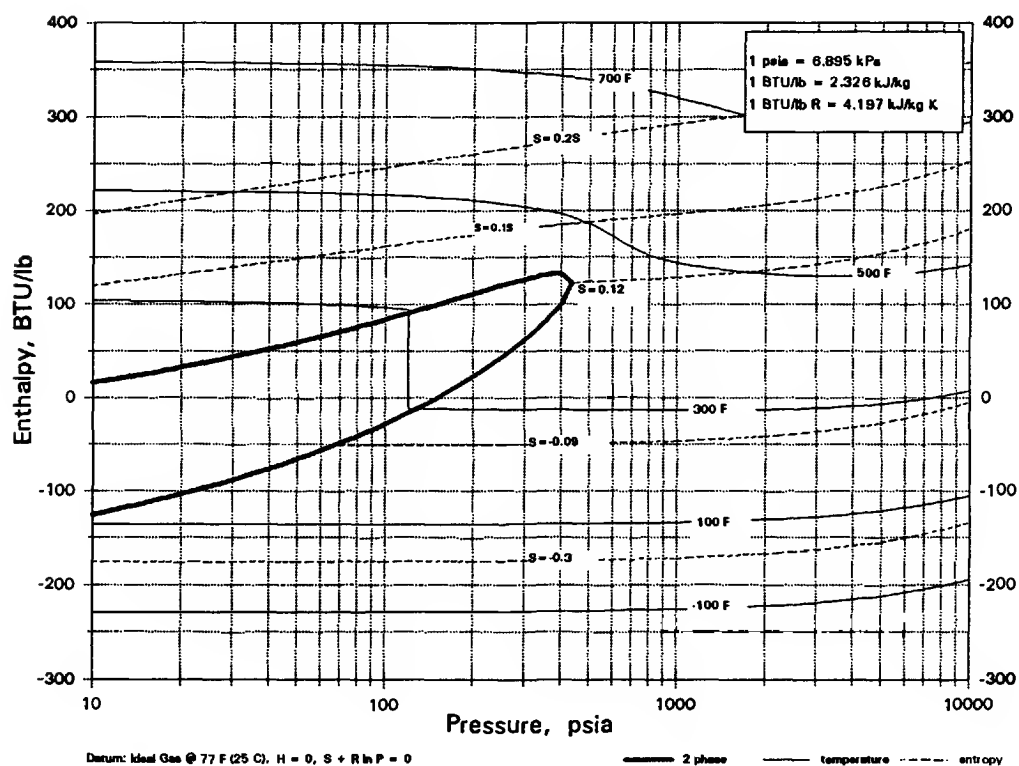


C6H14

n-HEXANE

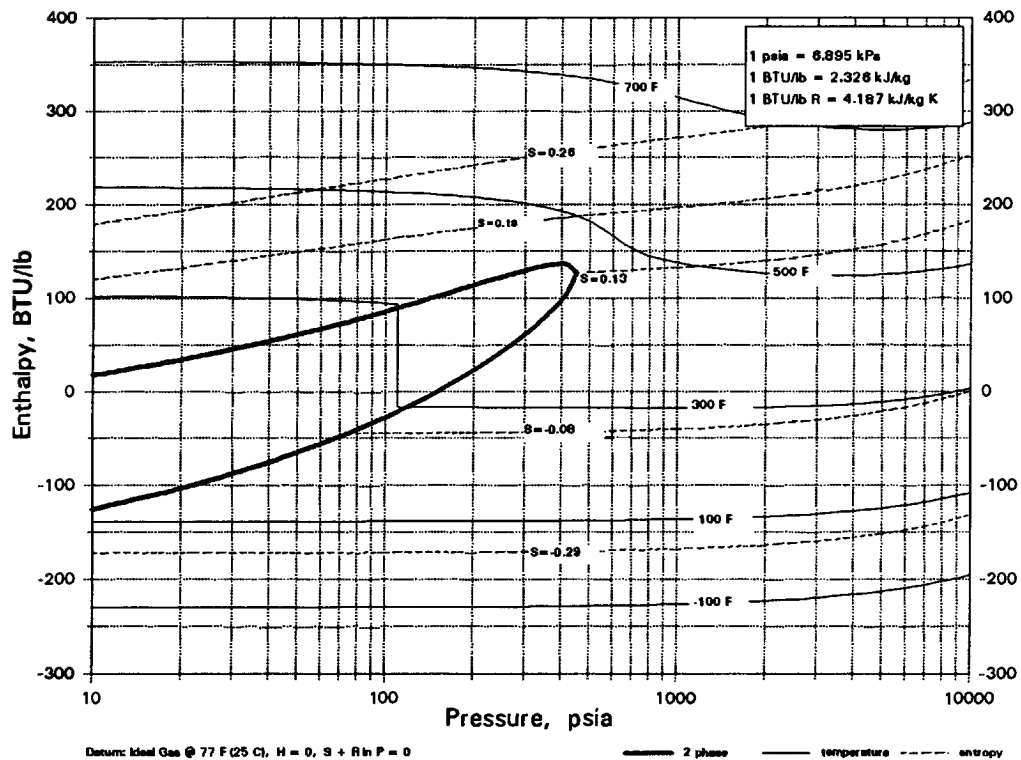
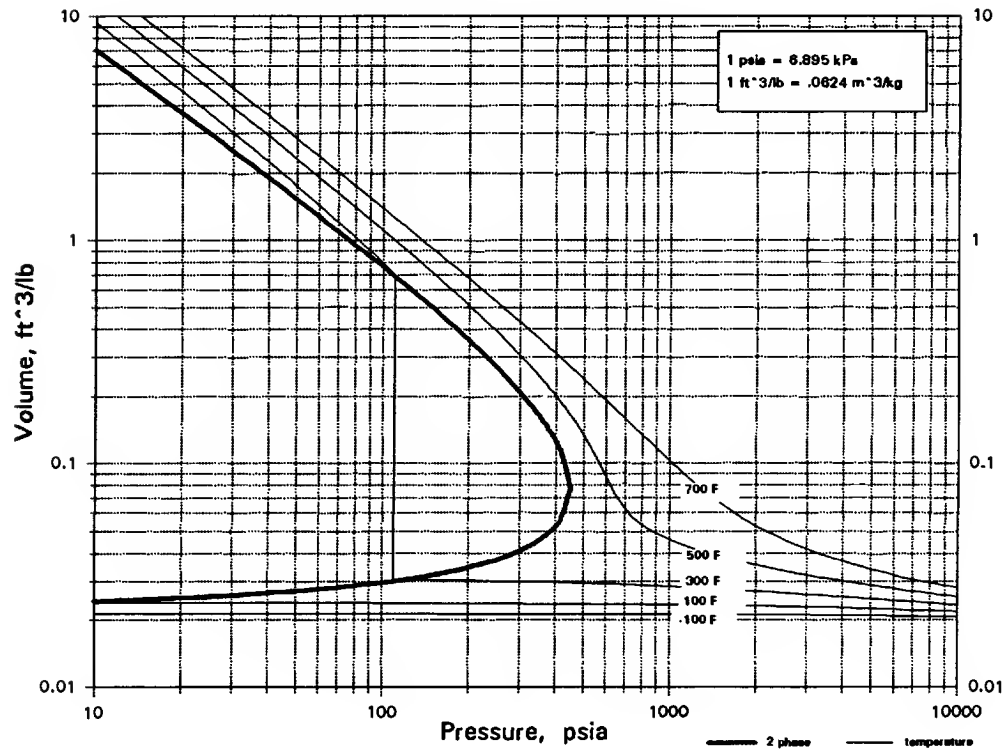


2-METHYLPENTANE

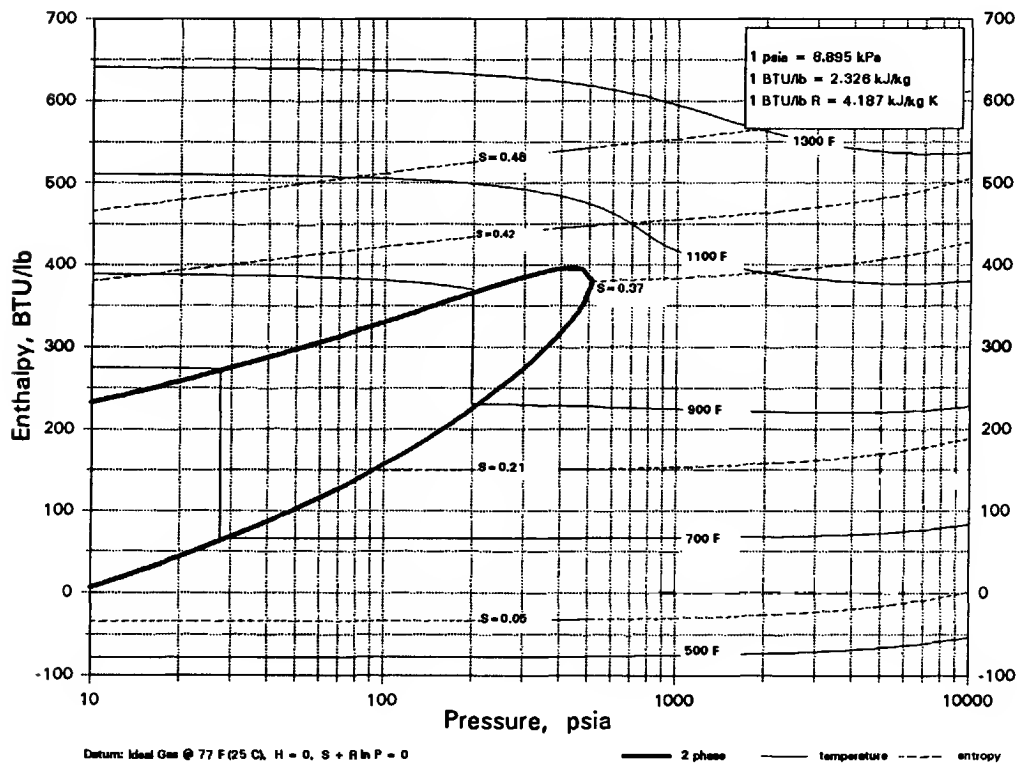
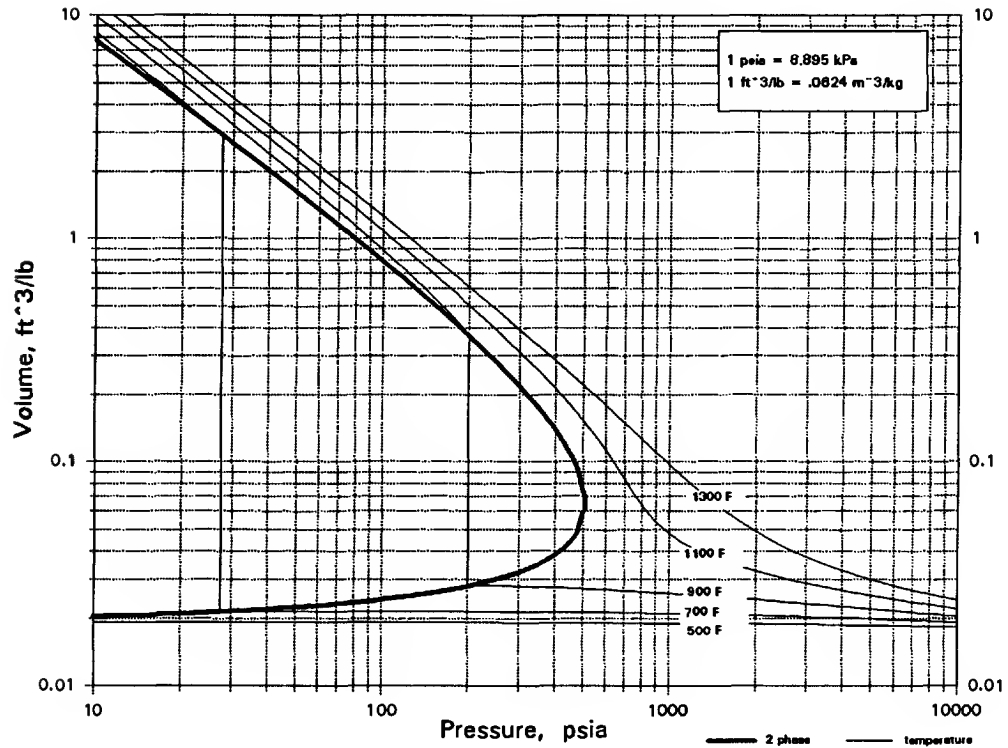


C6H14

3-METHYLPENTANE

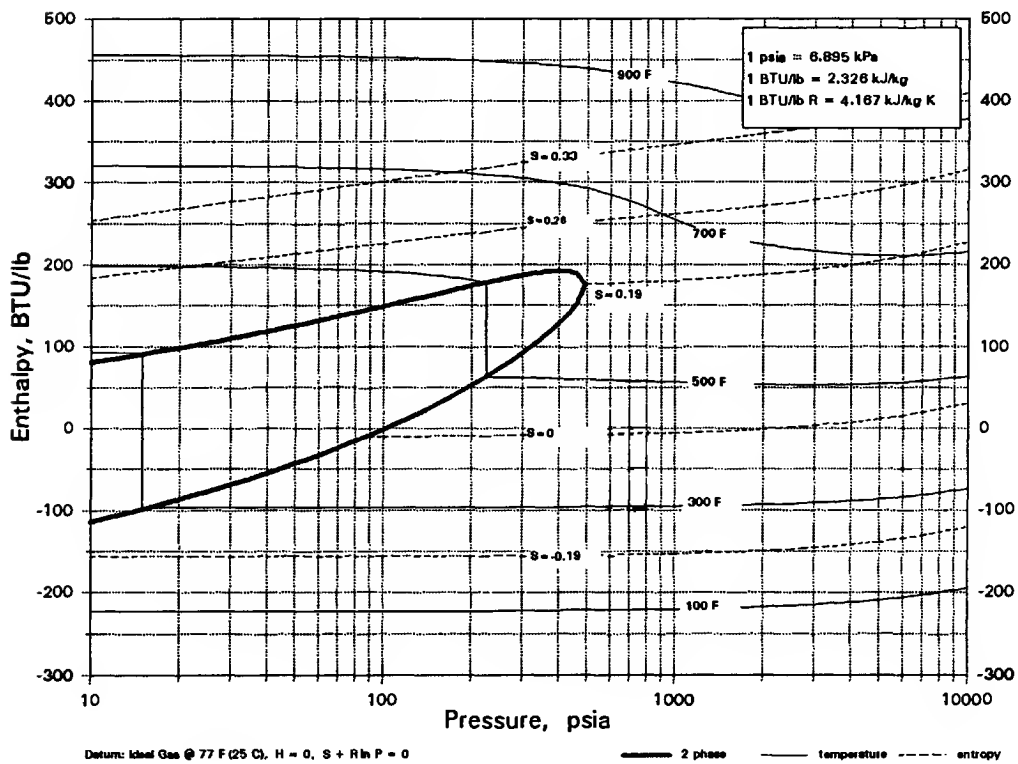
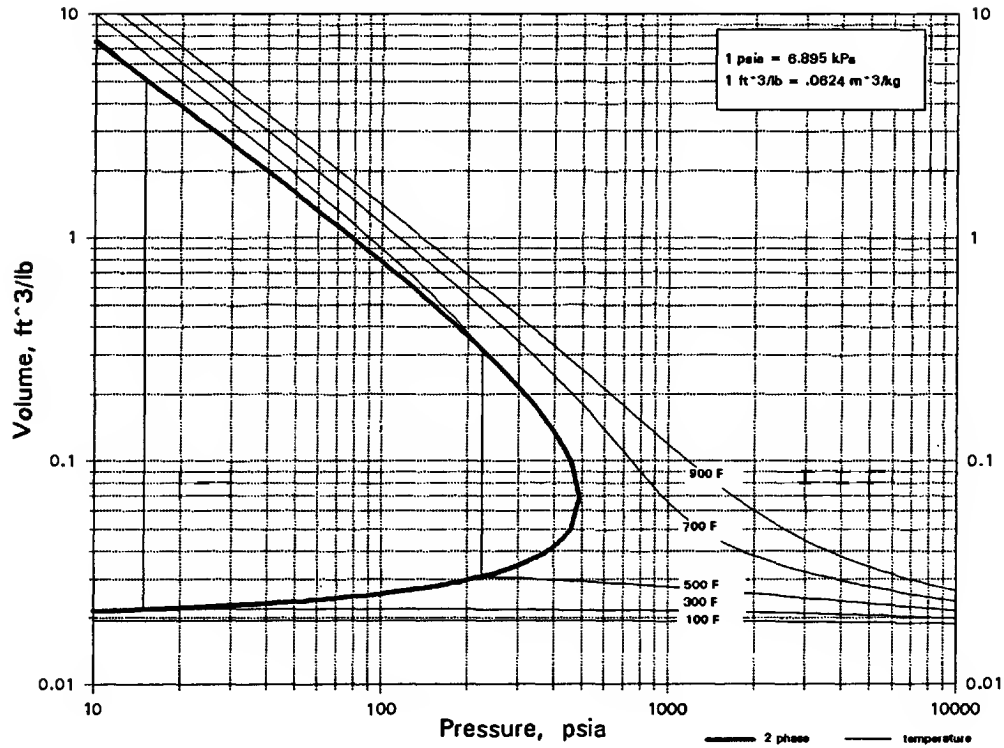


C6H14N2O2 LYSINE



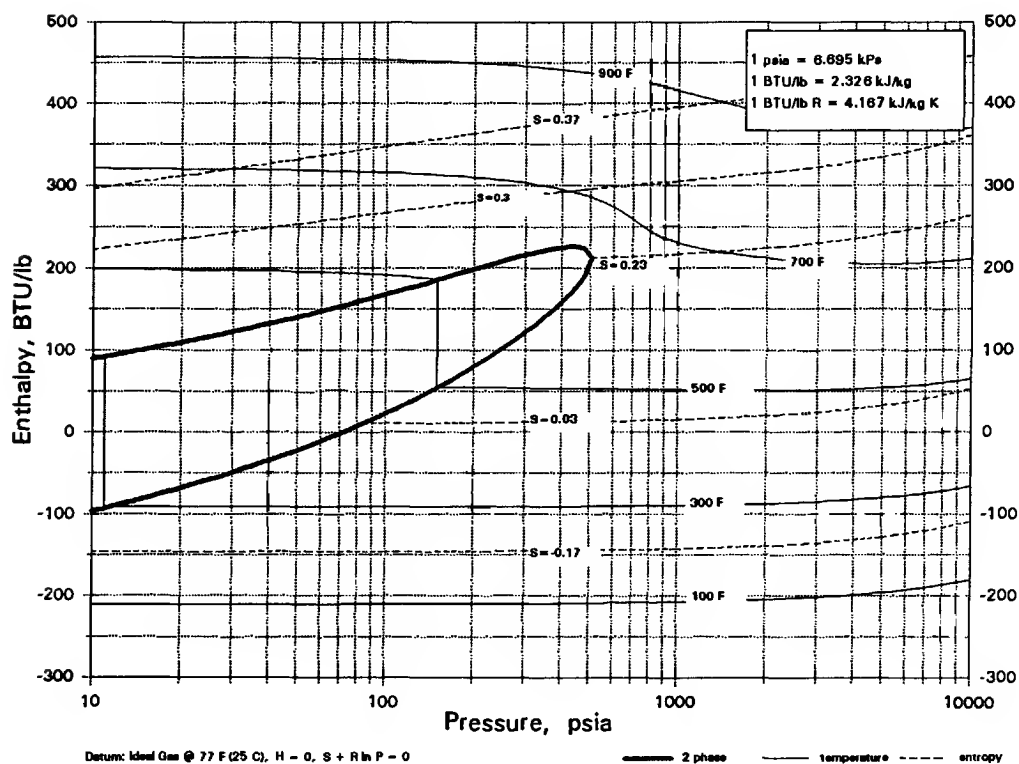
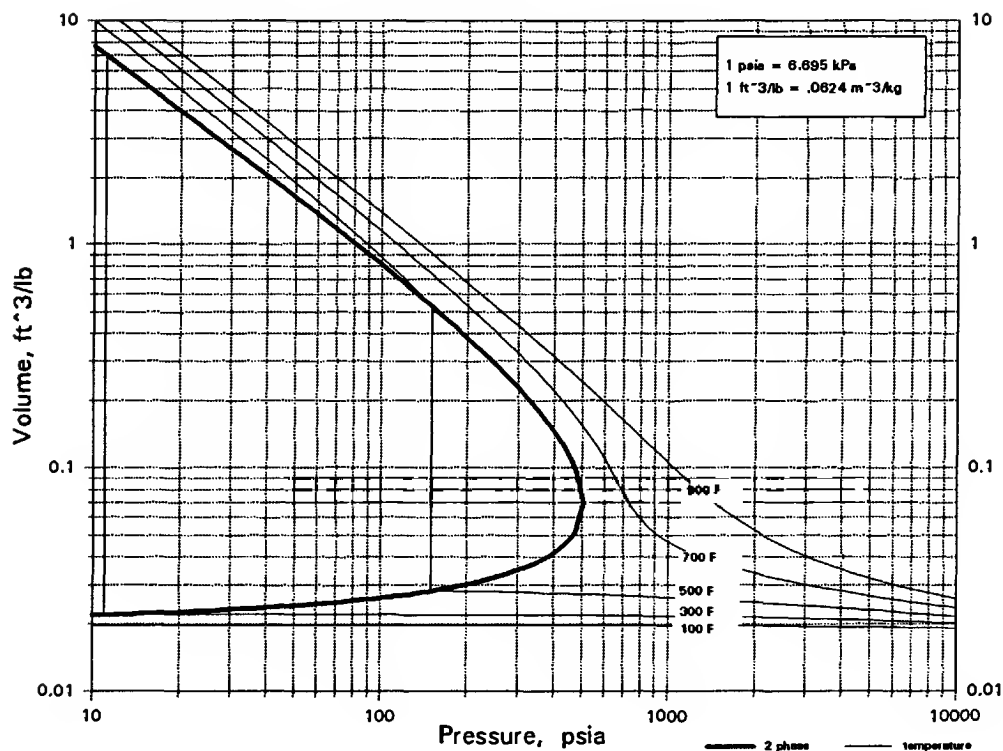
C6H14O

2-ETHYL-1-BUTANOL



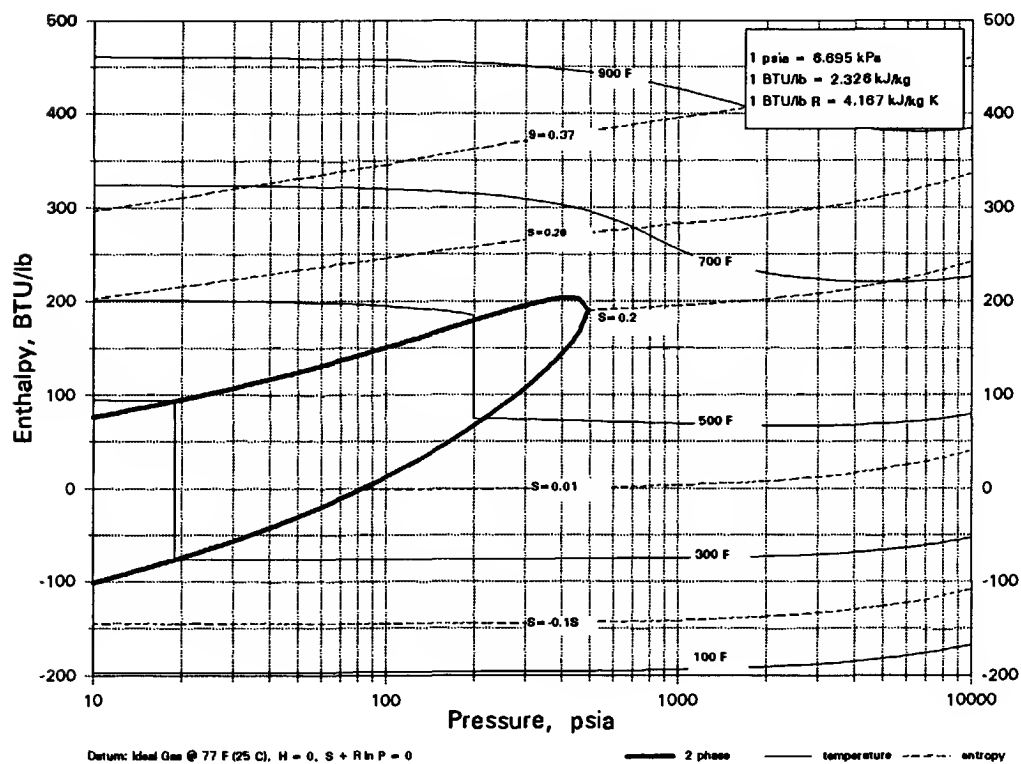
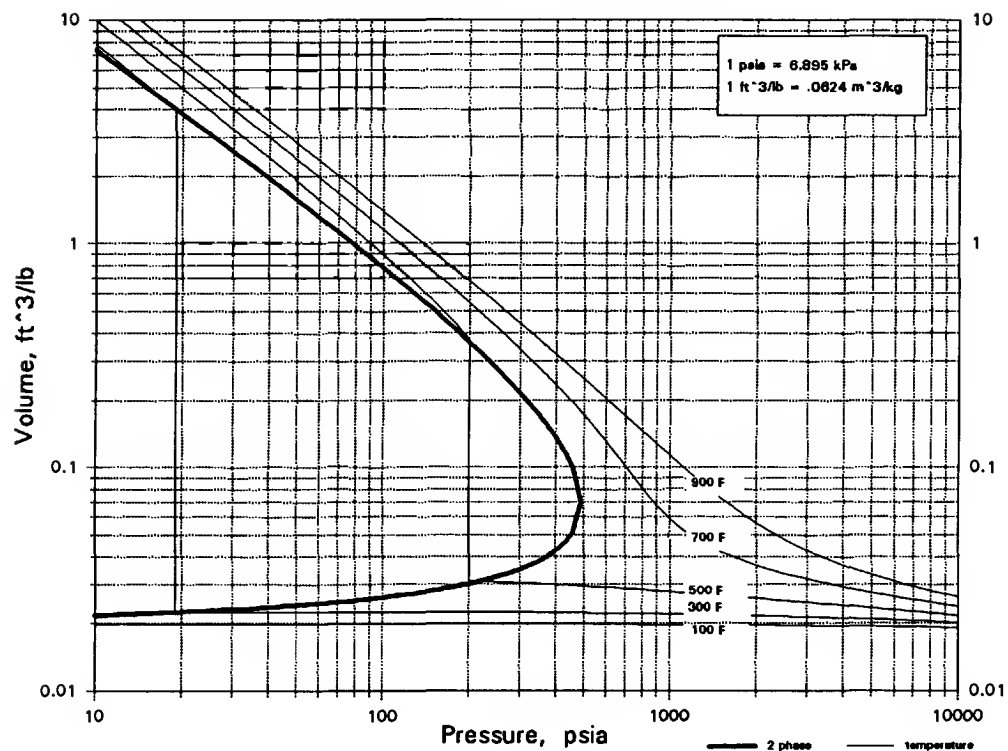
C6H14O

1-HEXANOL



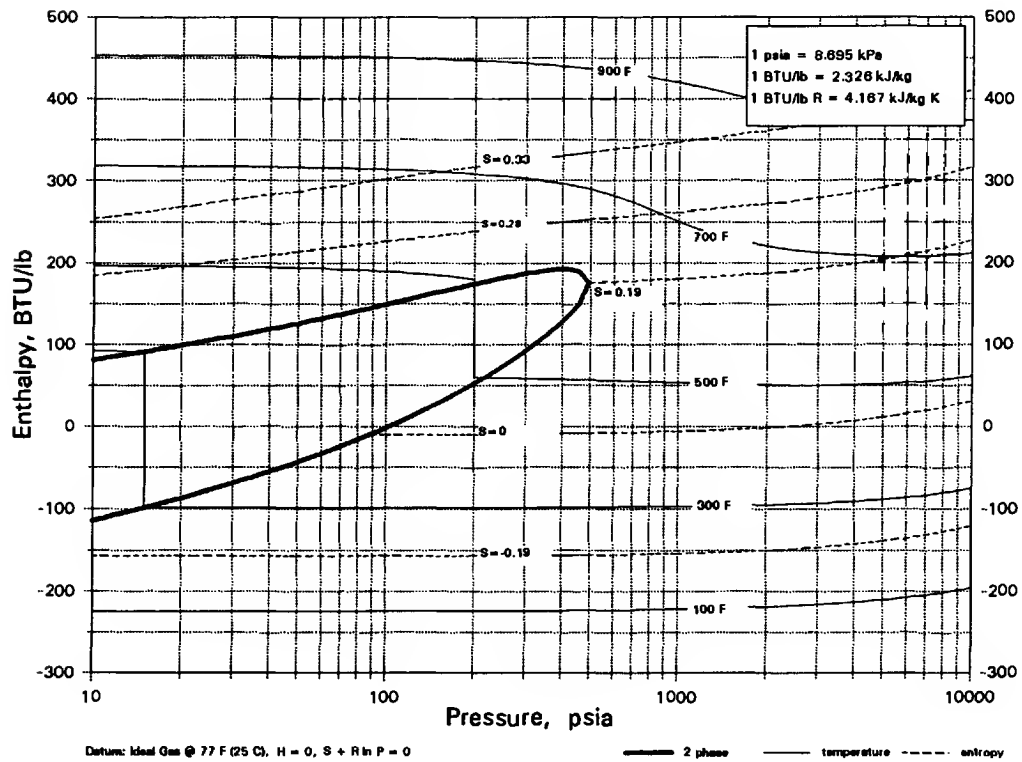
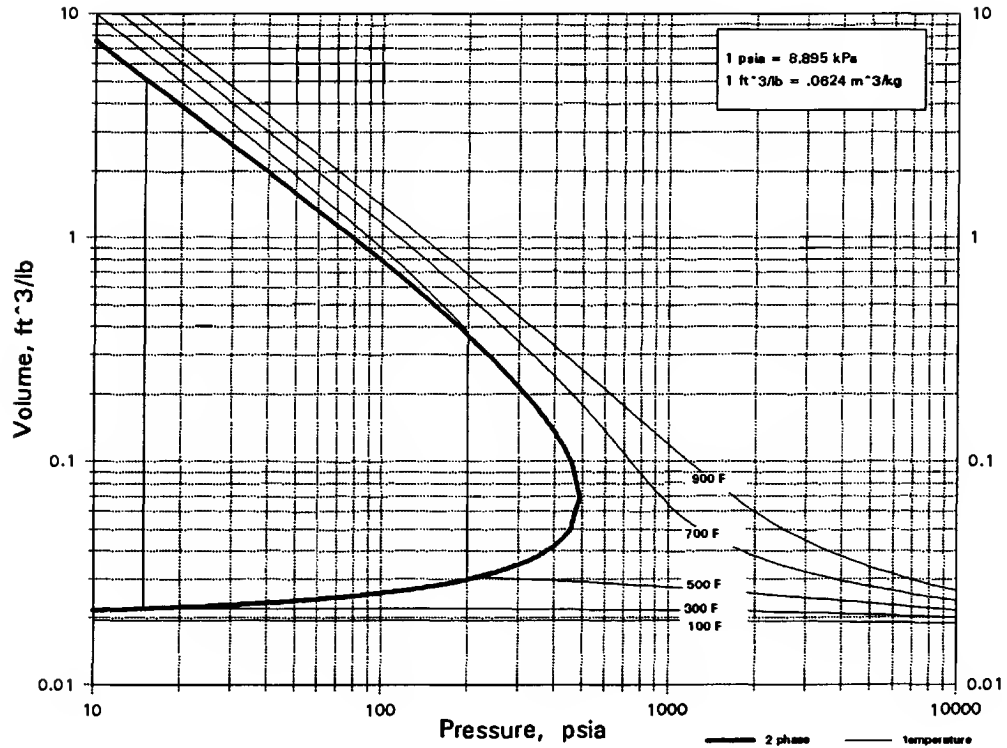
C6H14O

2-HEXANOL



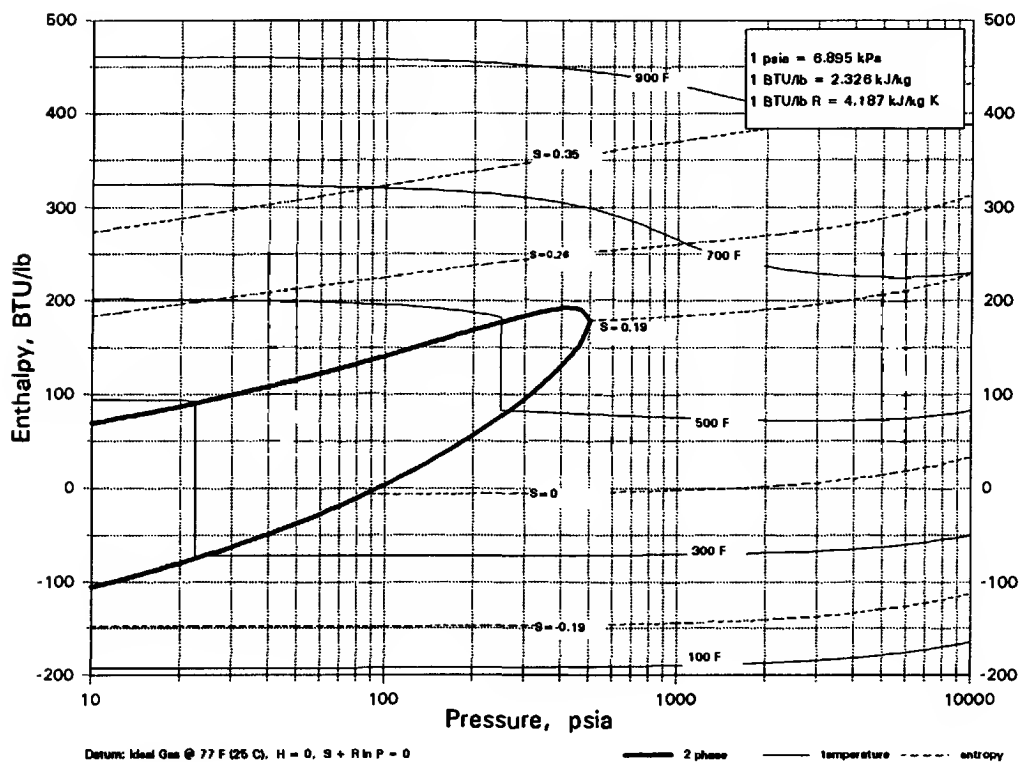
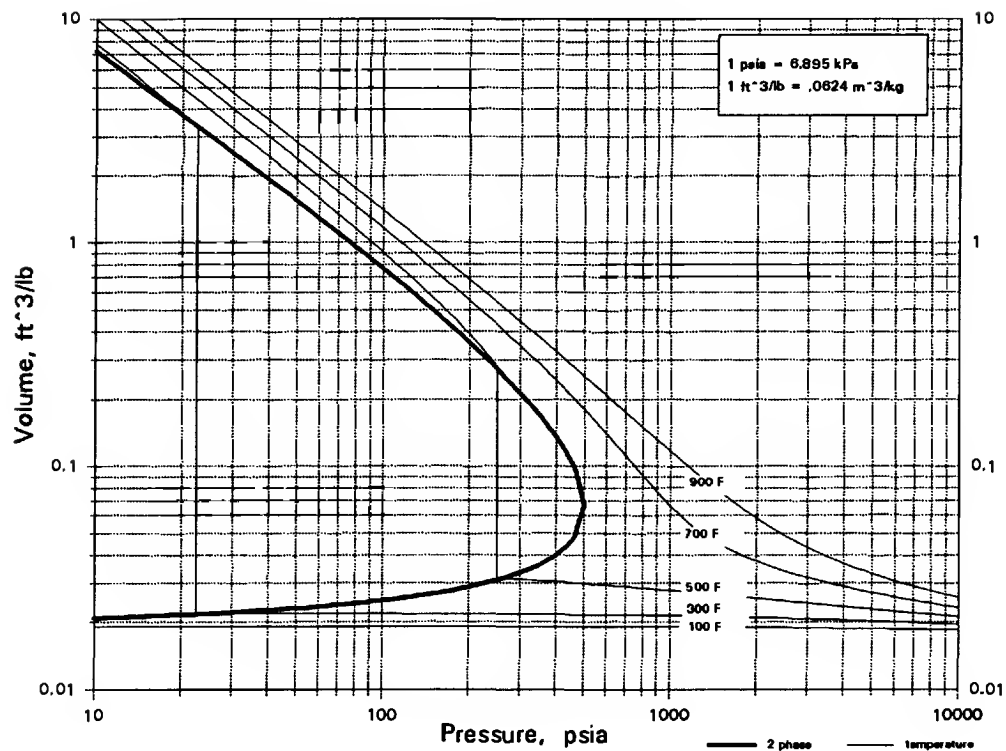
C6H14O

2-METHYL-1-PENTANOL



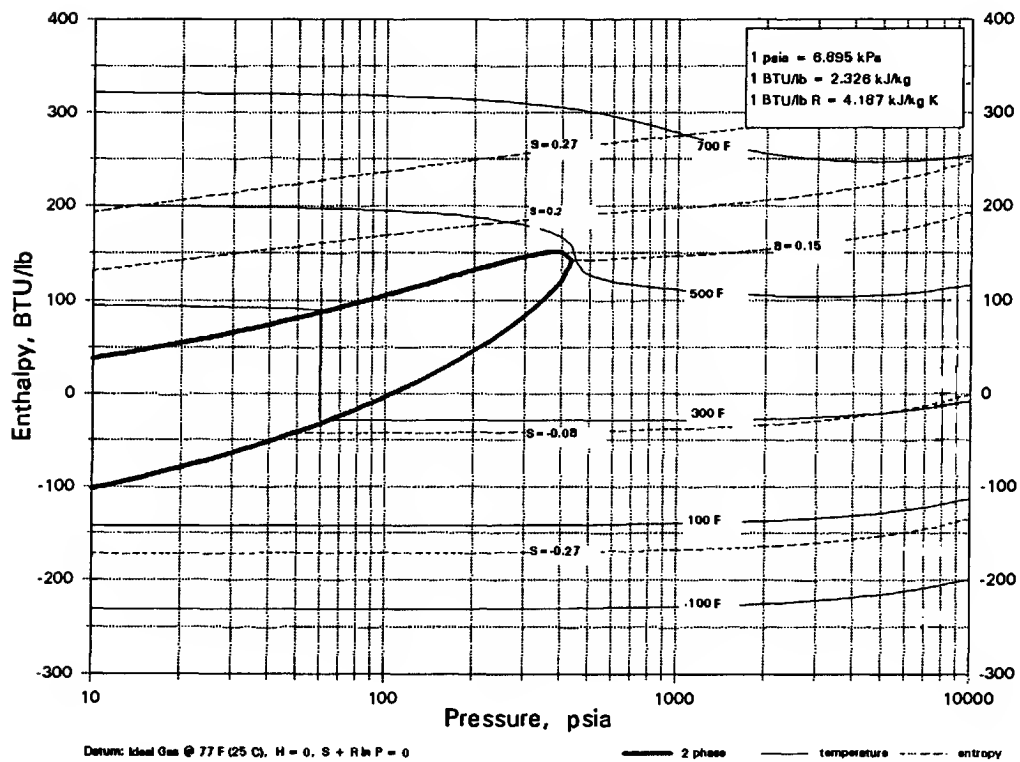
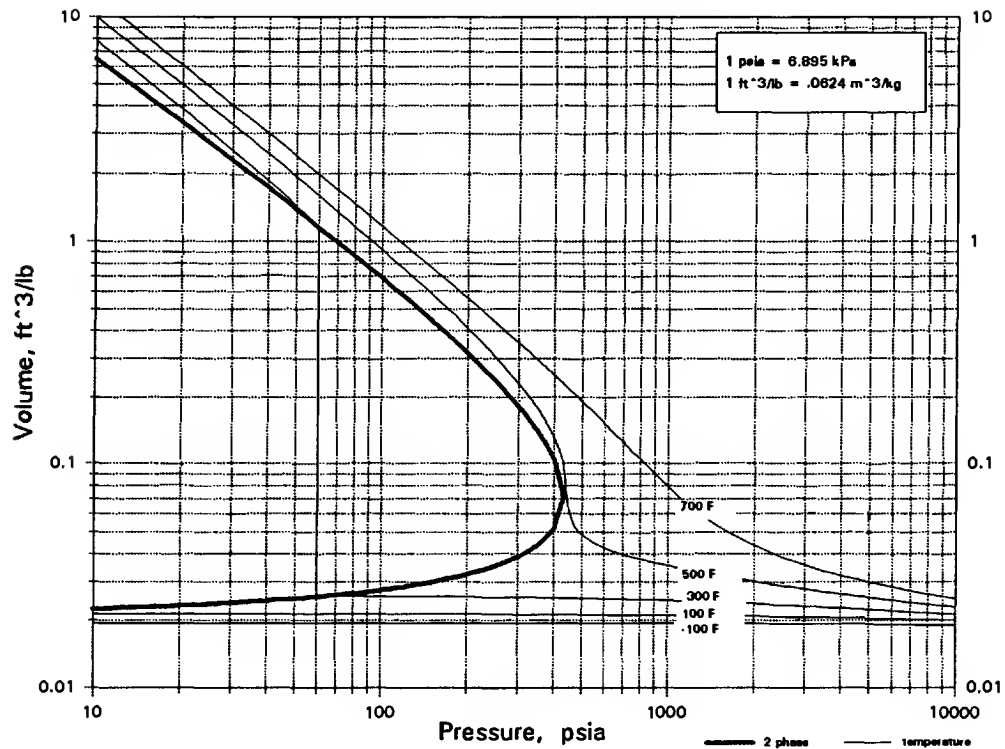
C6H14O

4-METHYL-2-PENTANOL



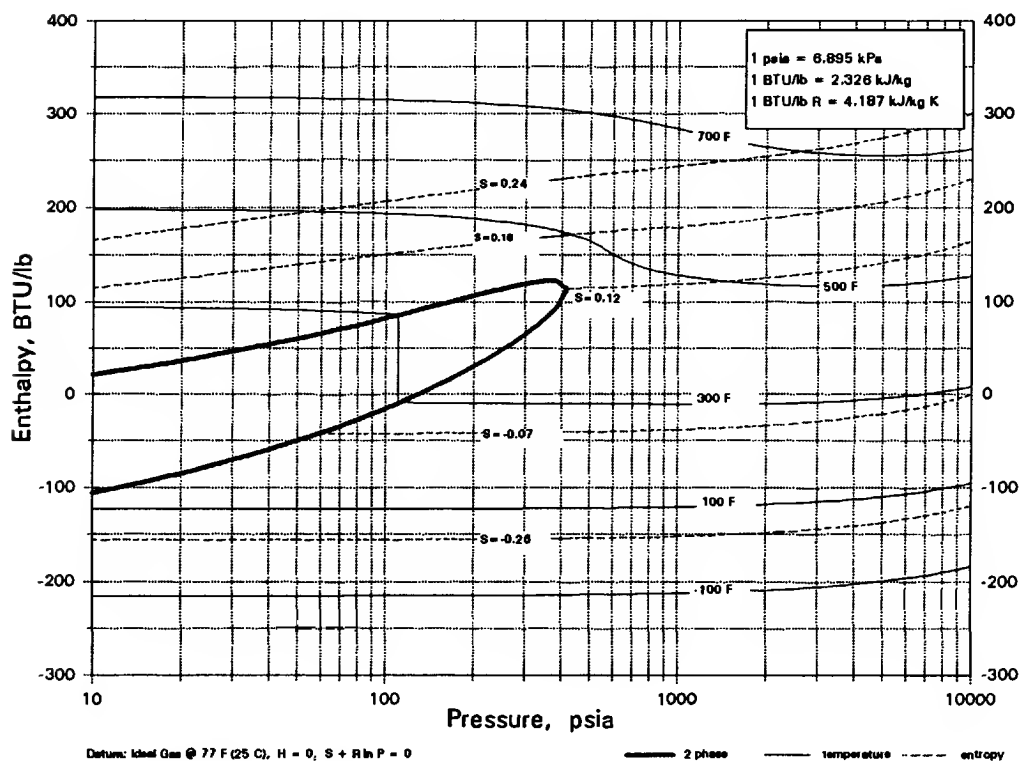
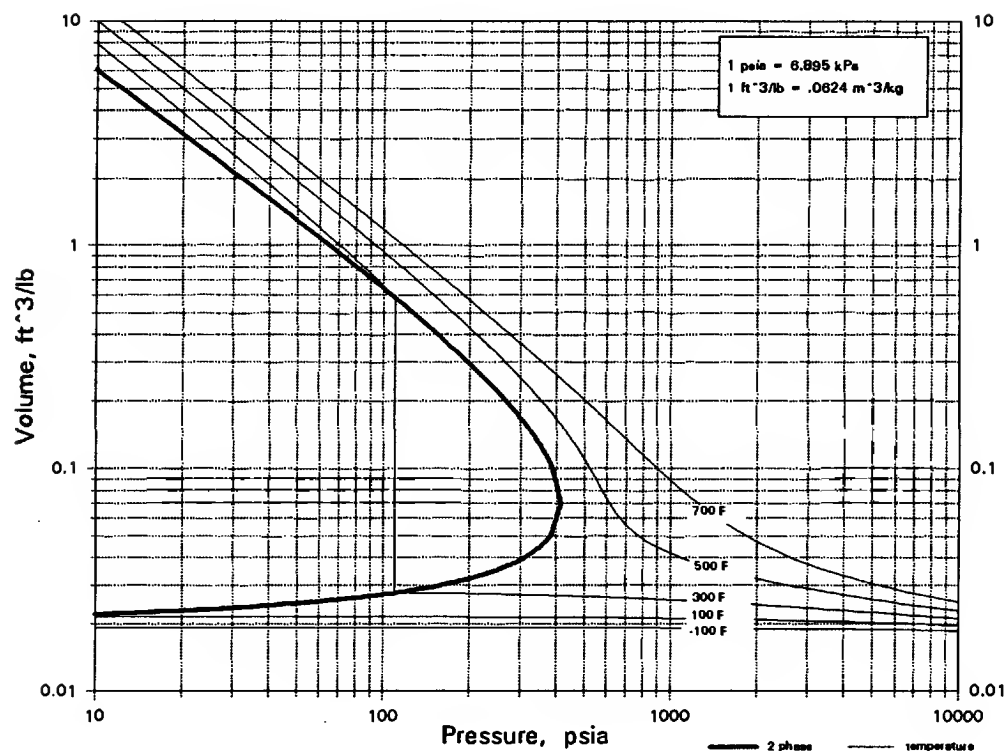
C6H14O

n-BUTYL ETHYL ETHER



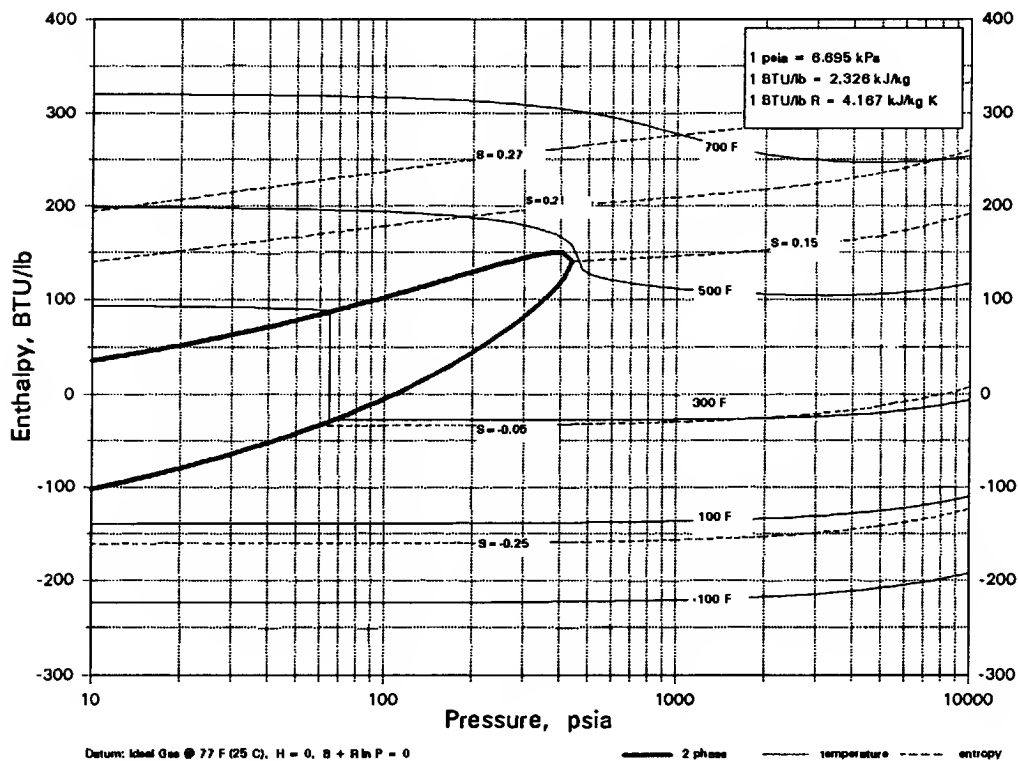
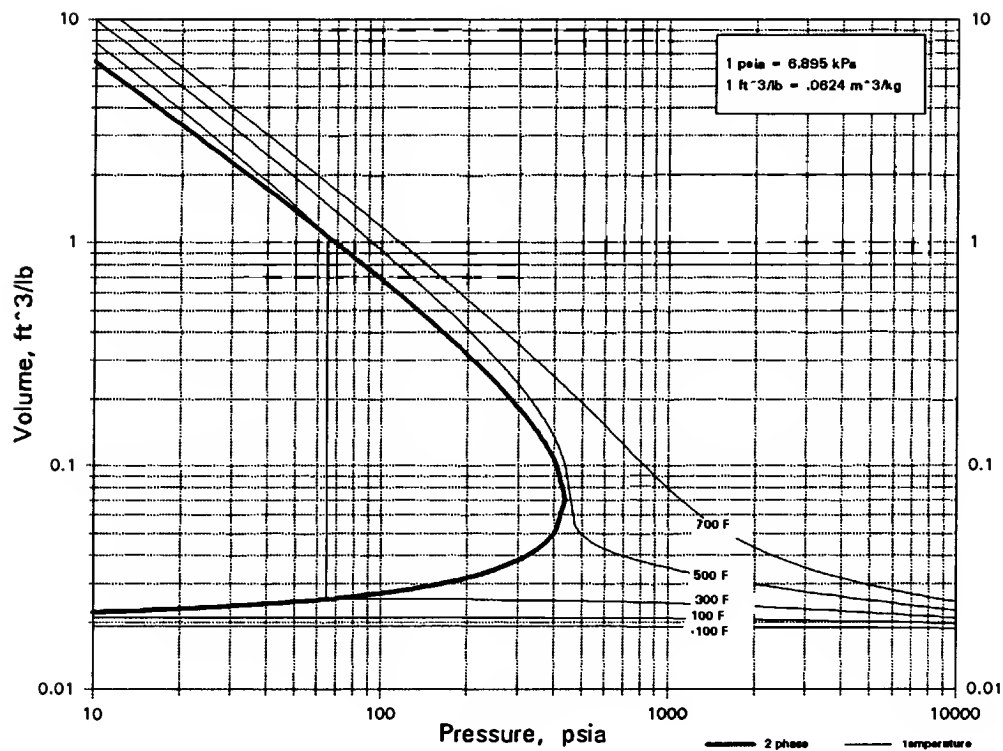
C6H14O

DIISOPROPYL ETHER



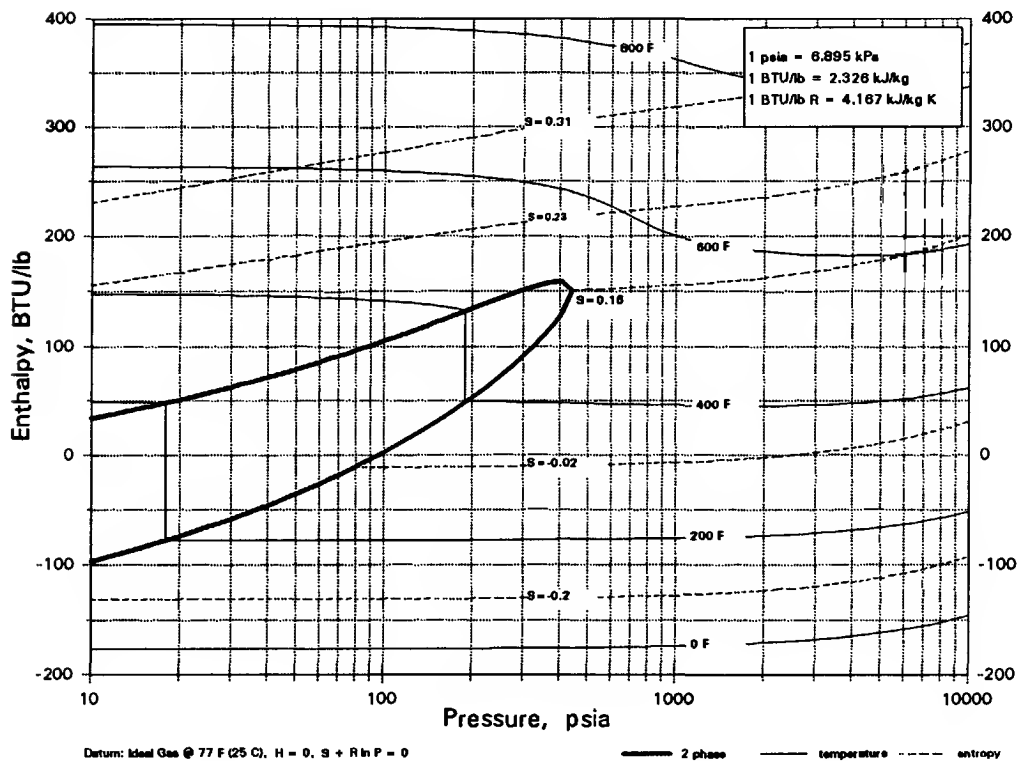
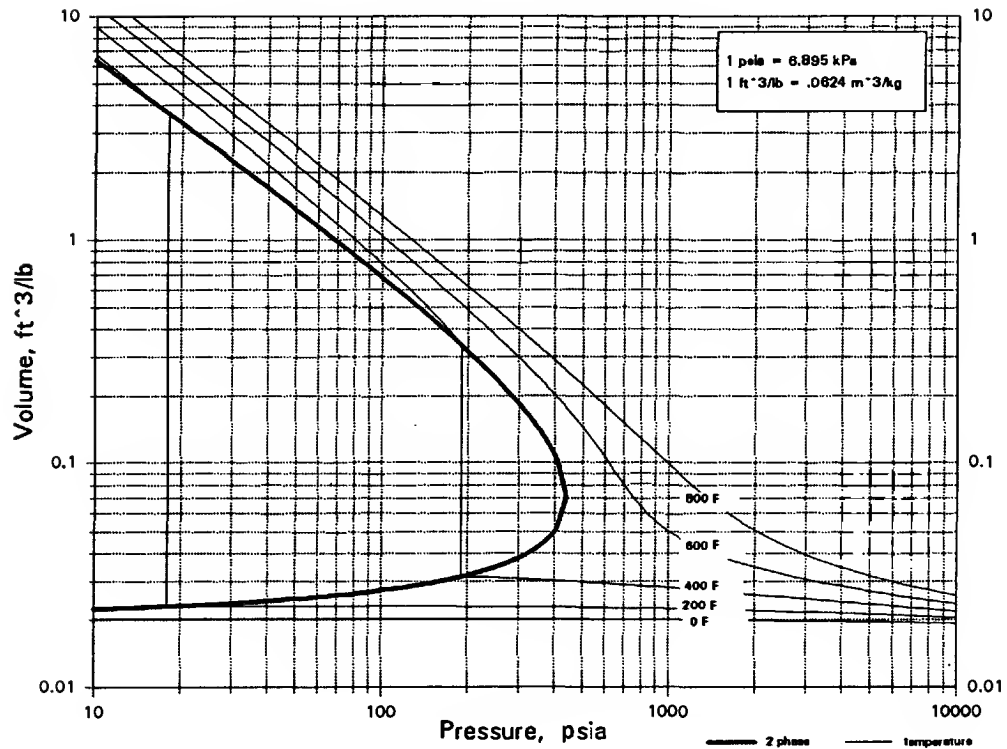
C6H14O

DI-n-PROPYL ETHER



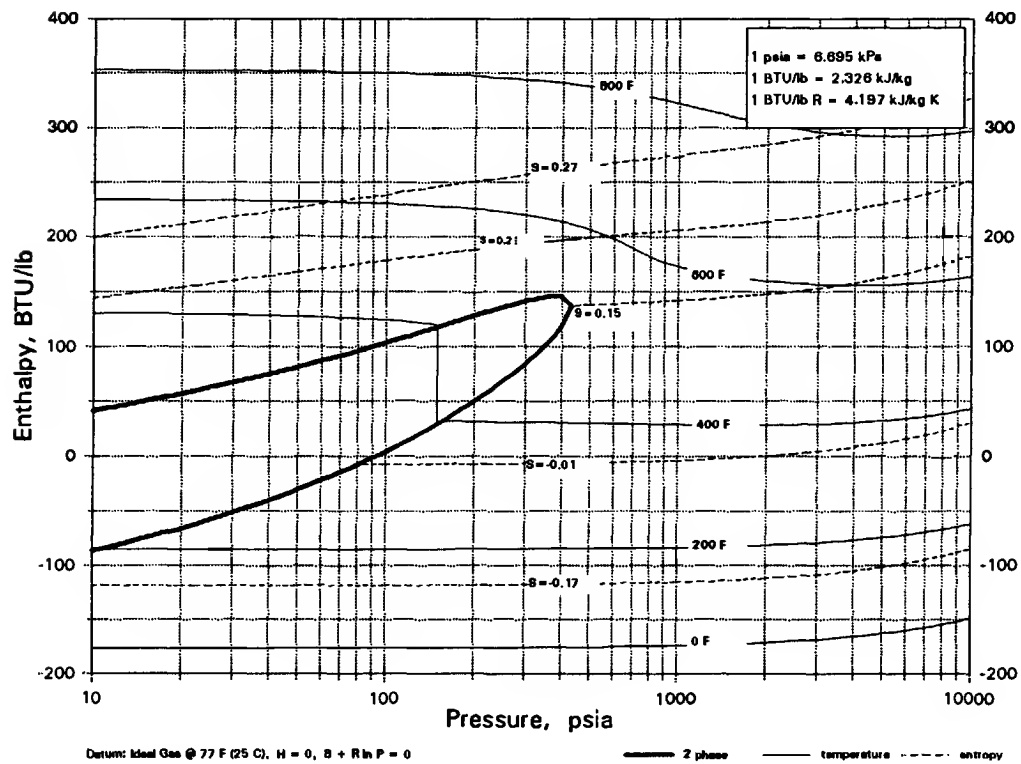
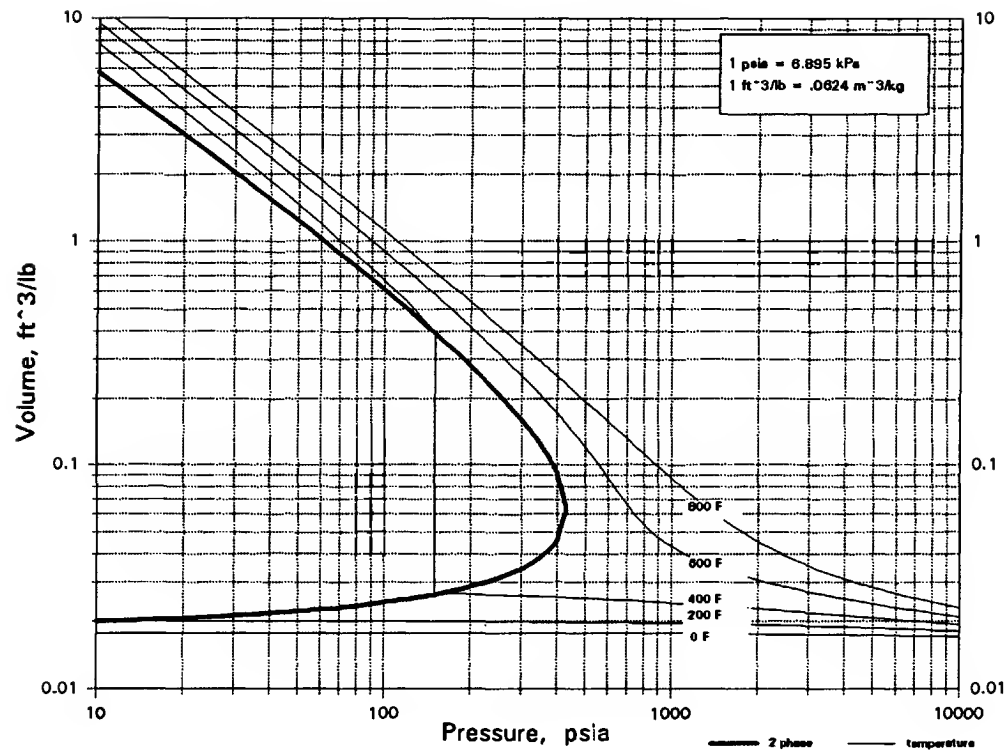
C6H14O

METHYL tert-PENTYL ETHER



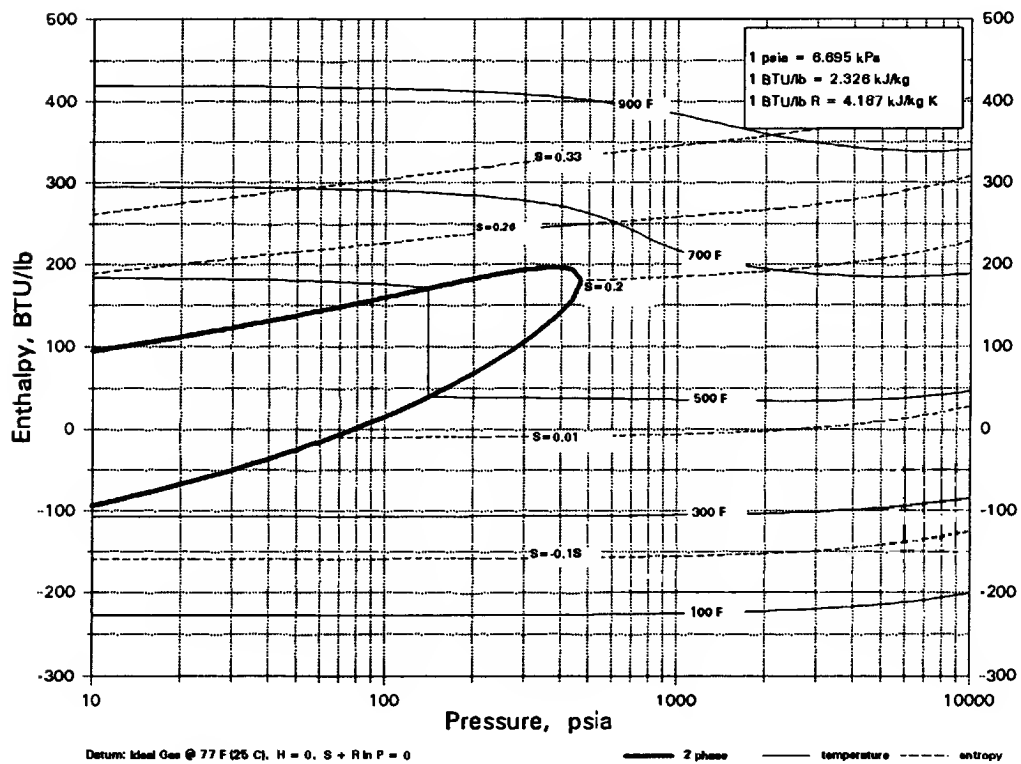
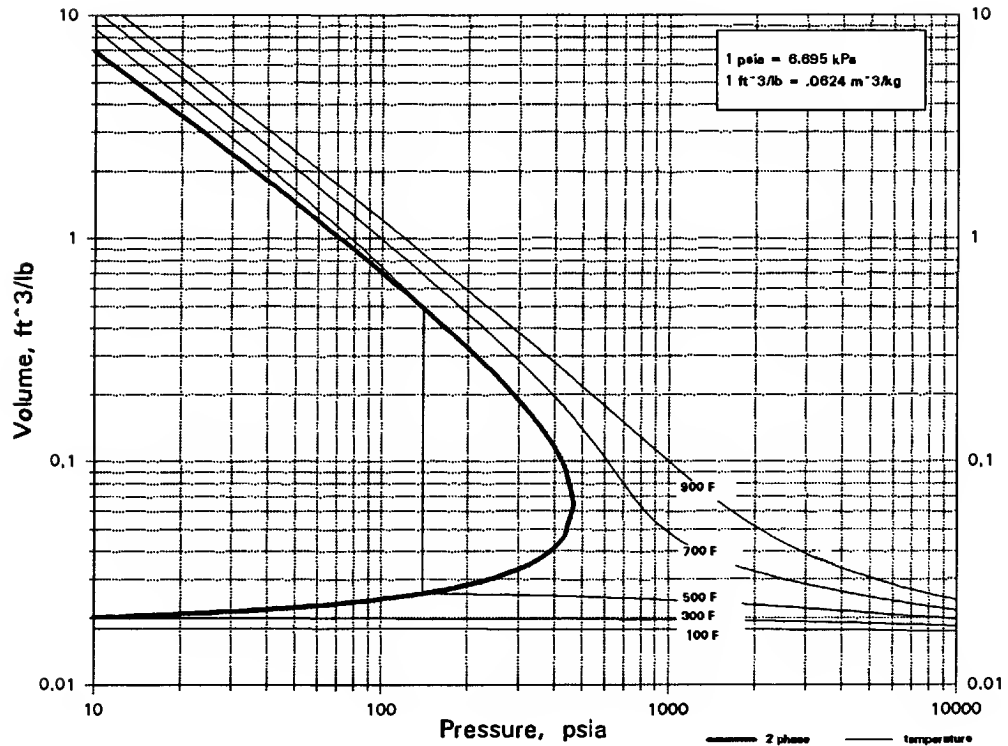
C6H14O2

ACETAL



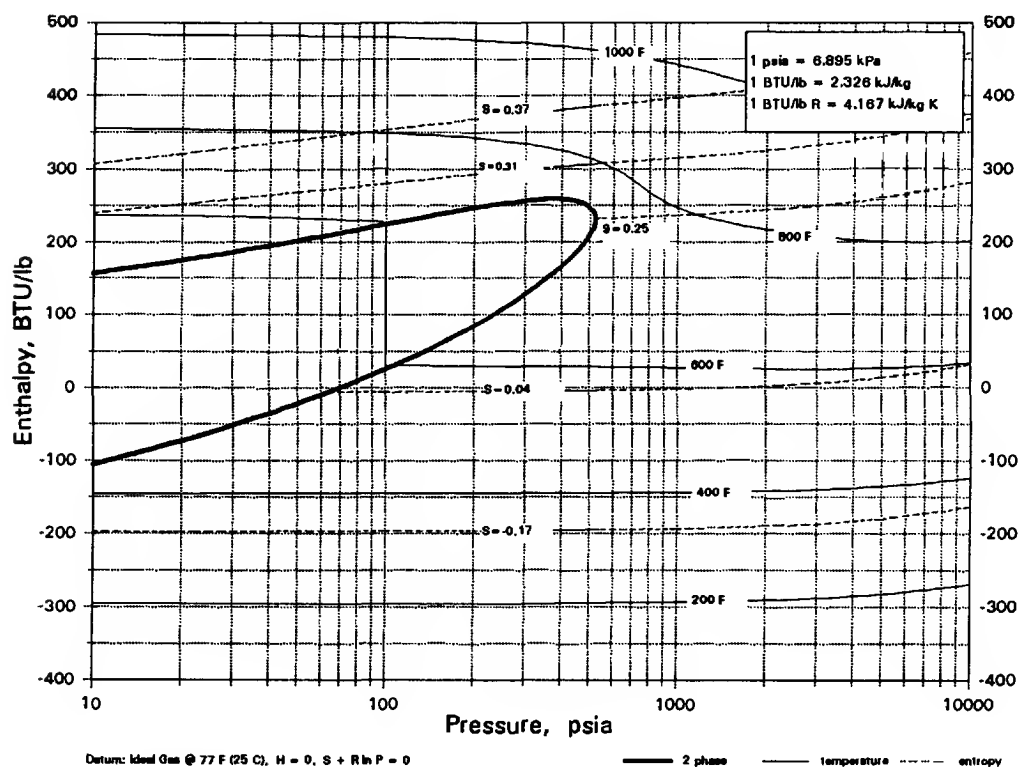
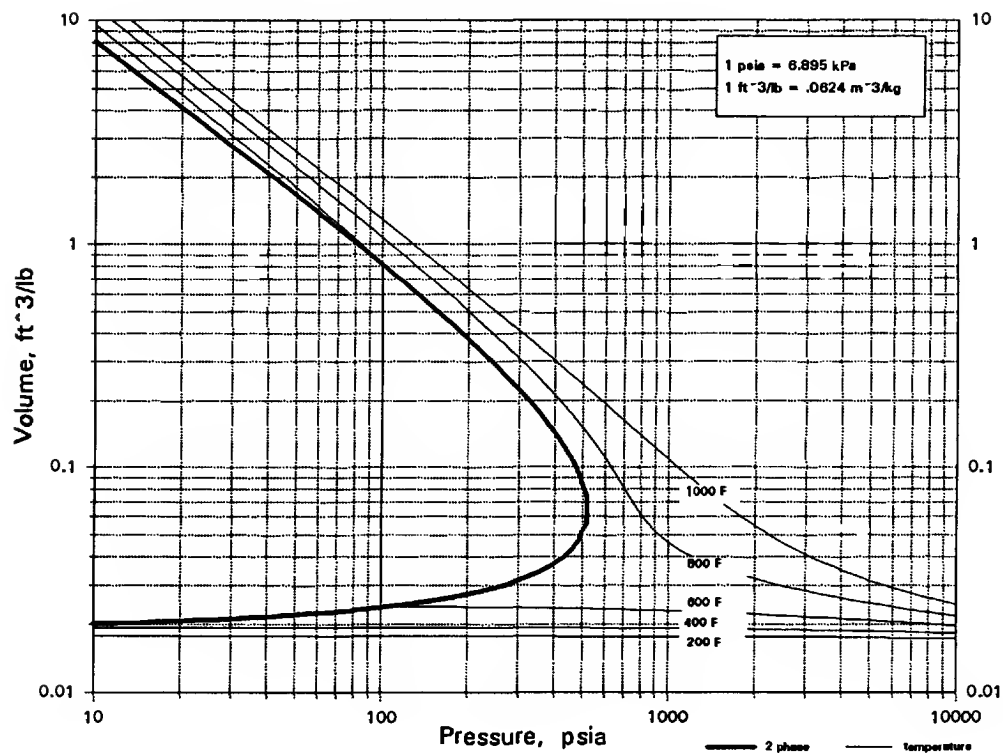
C6H14O2

2-BUTOXYETHANOL



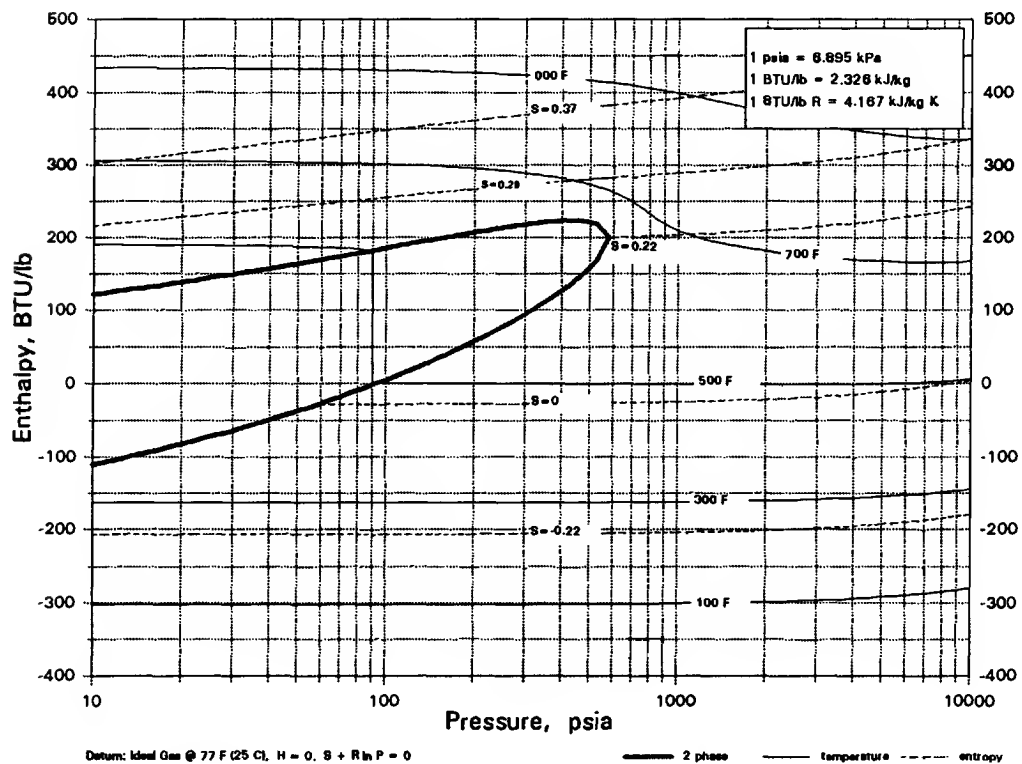
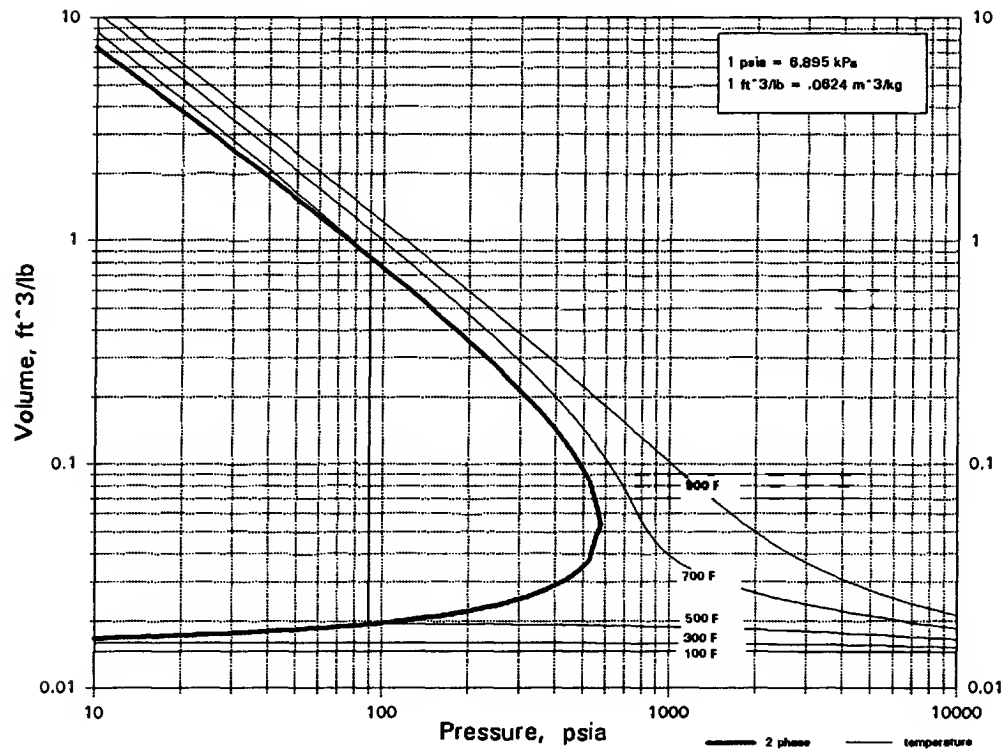
C6H14O2

1-6-HEXANEDIOL



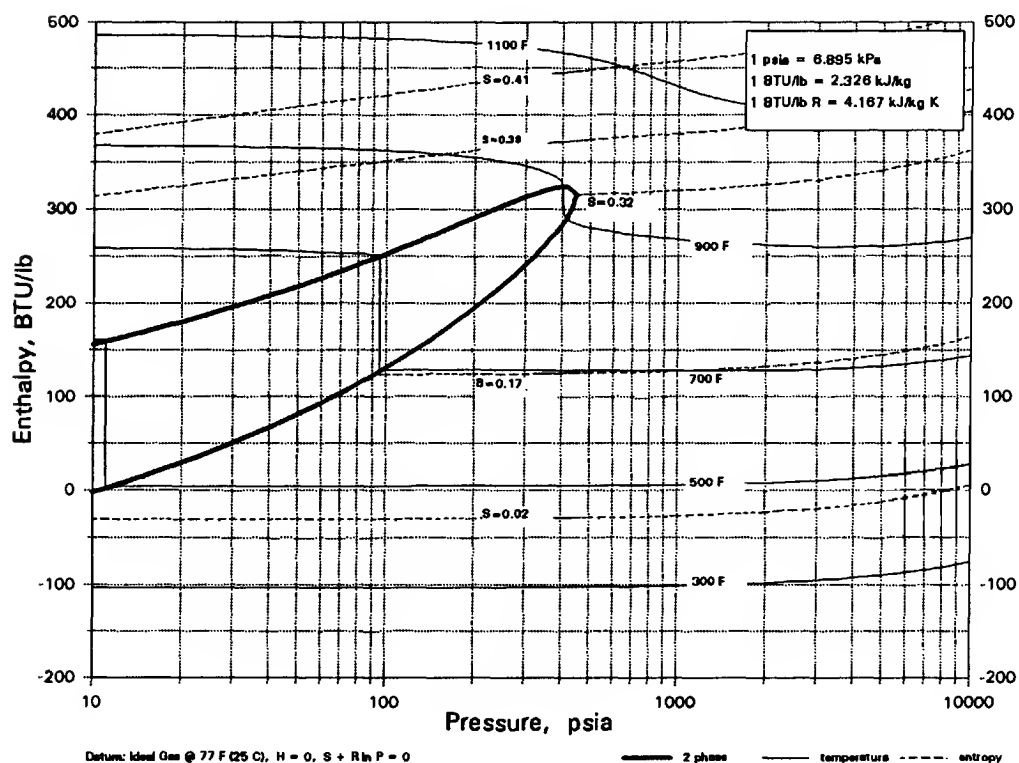
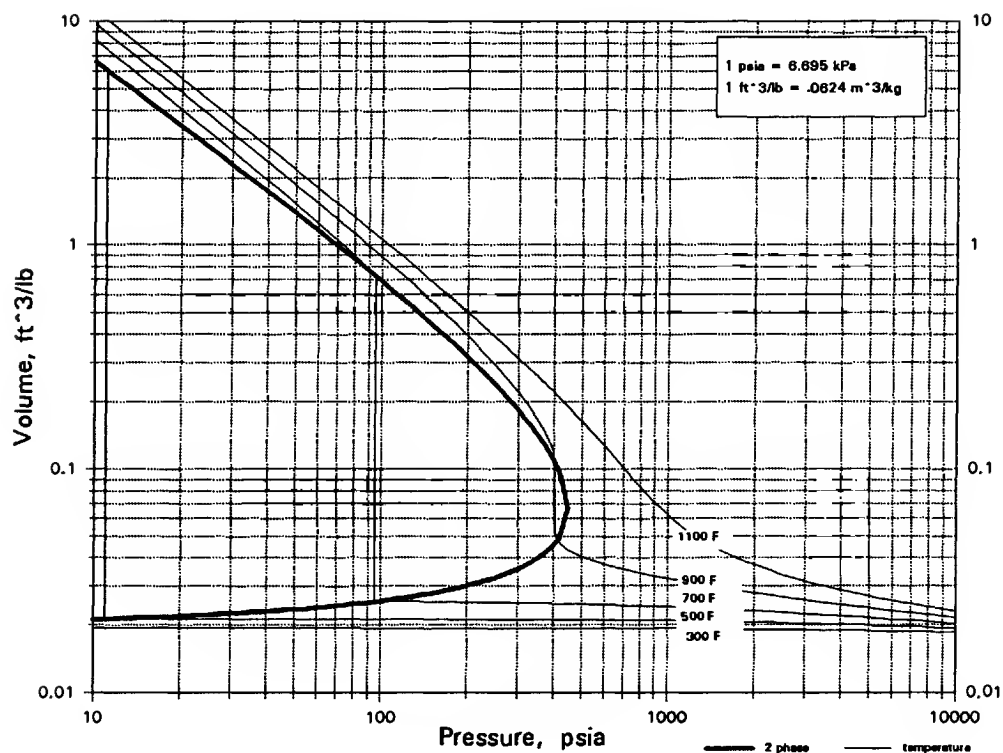
C6H14O2

HEXYLENE GLYCOL



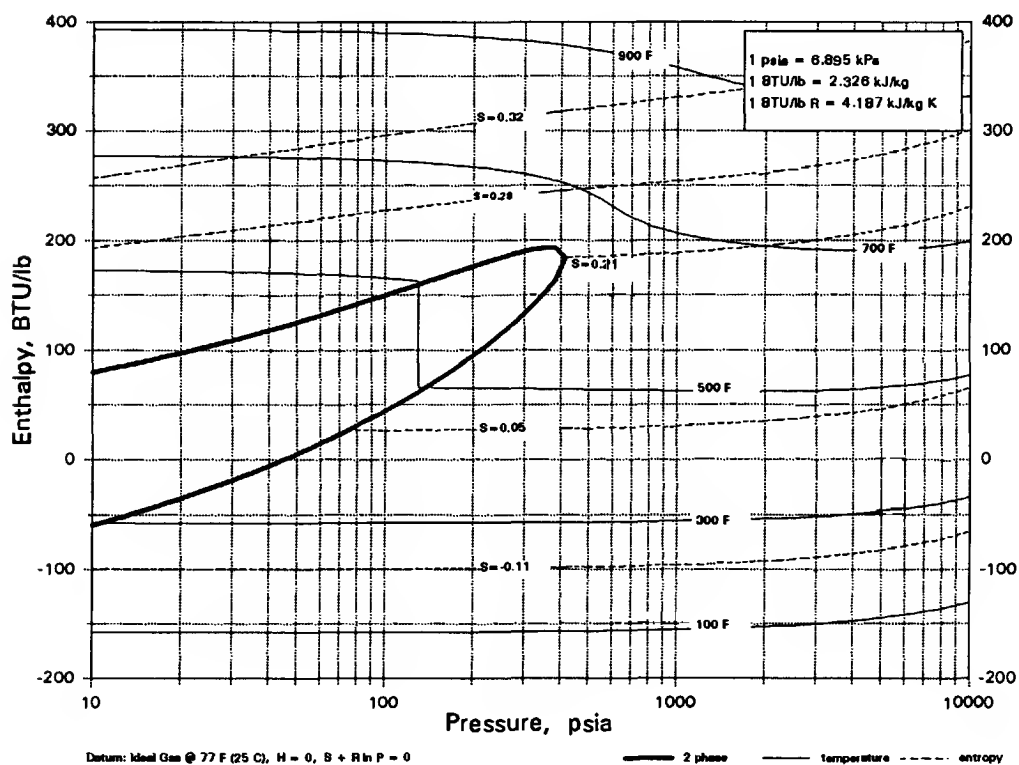
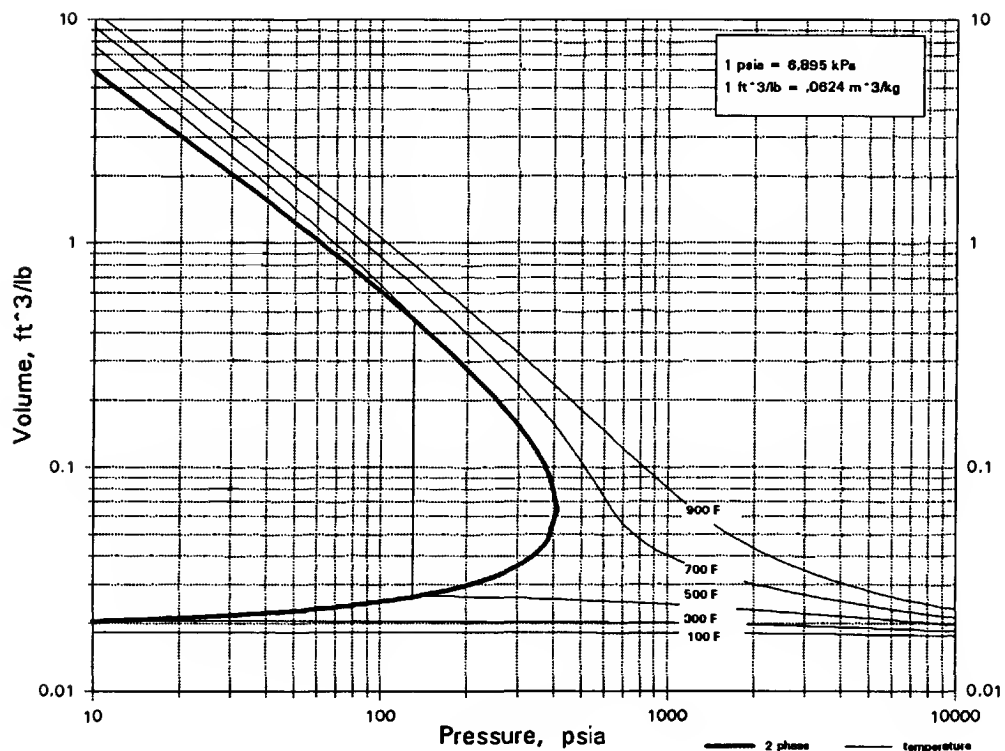
C6H14O2S

DI-n-PROPYL SULFONE

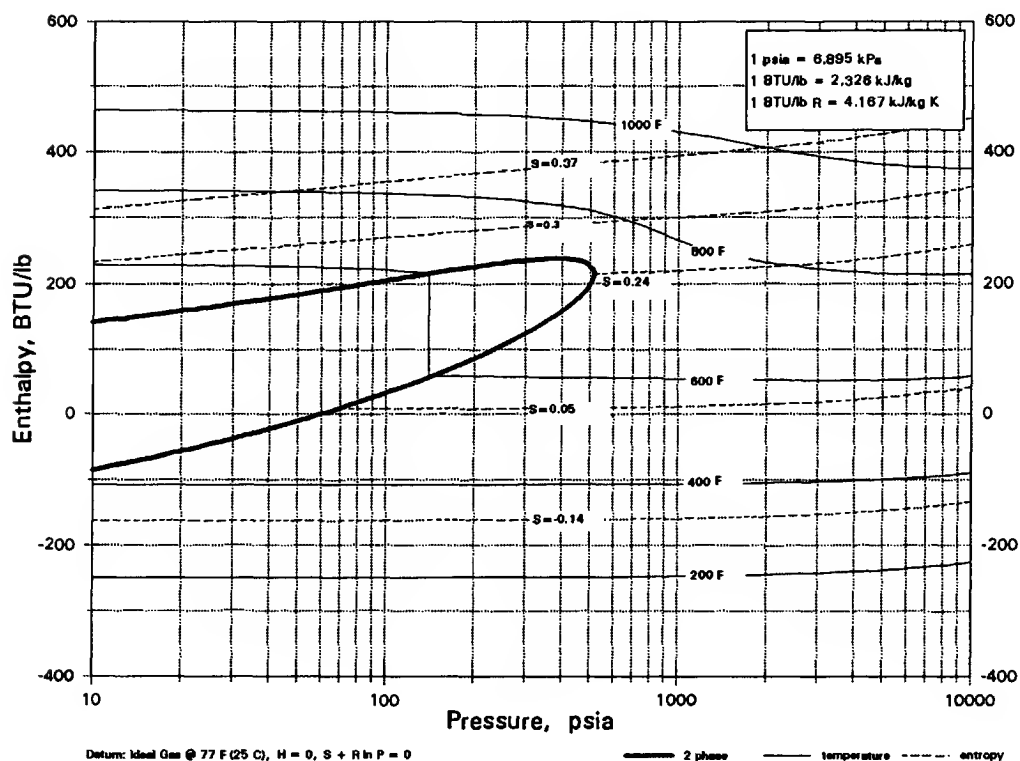
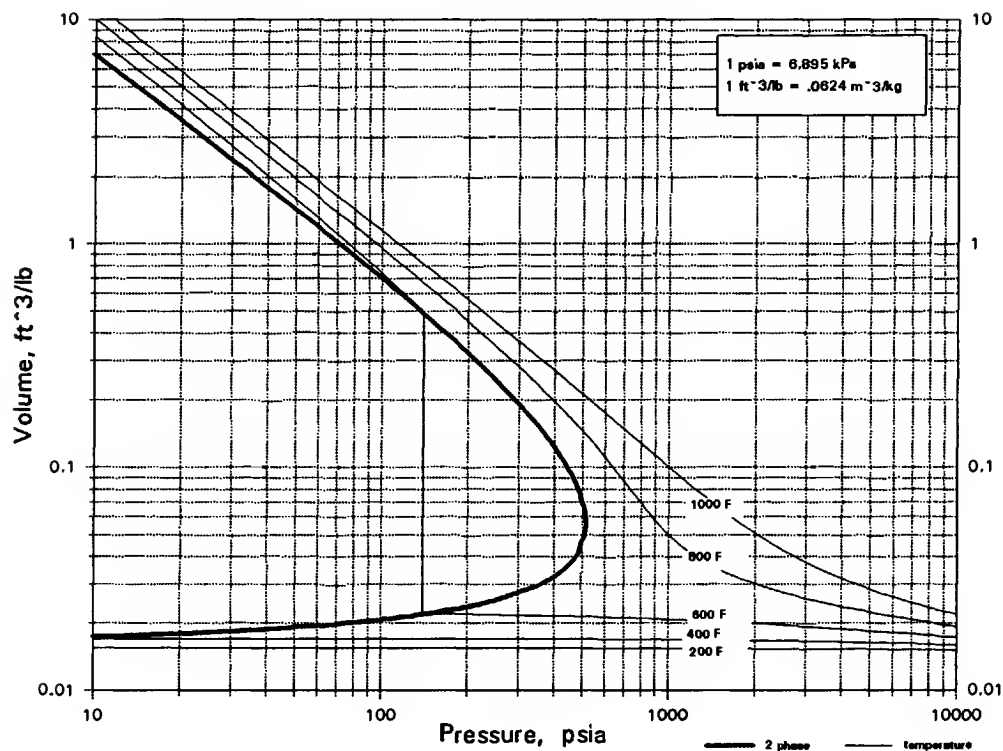


C6H14O3

DIETHYLENE GLYCOL DIMETHYL ETHER

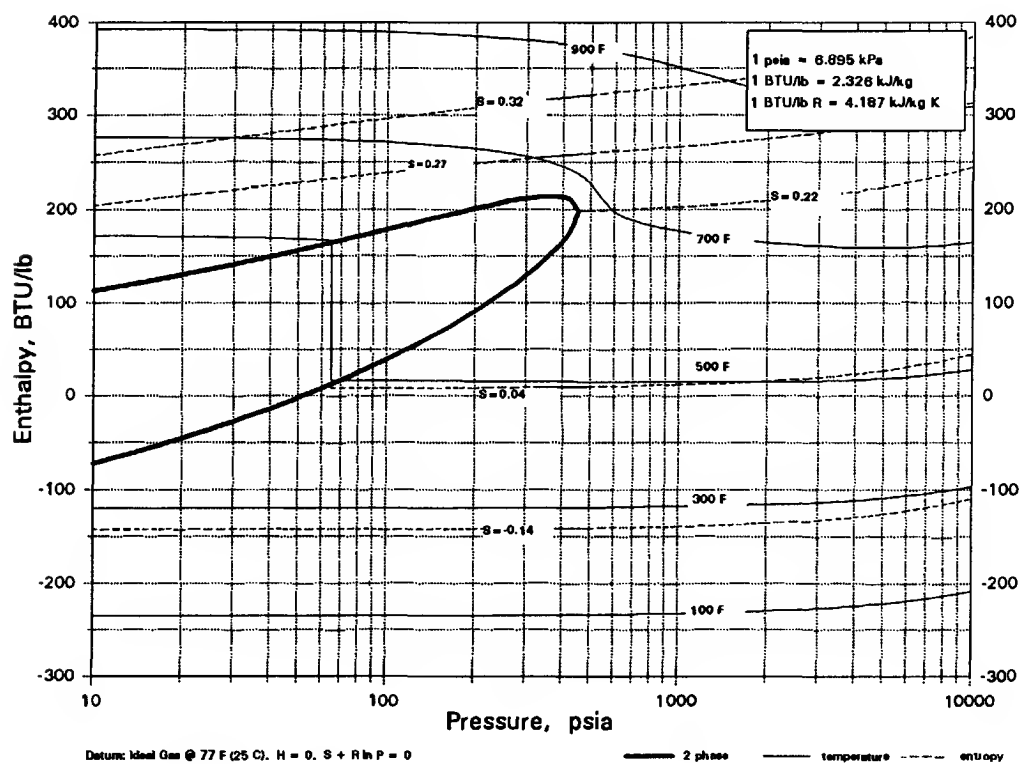
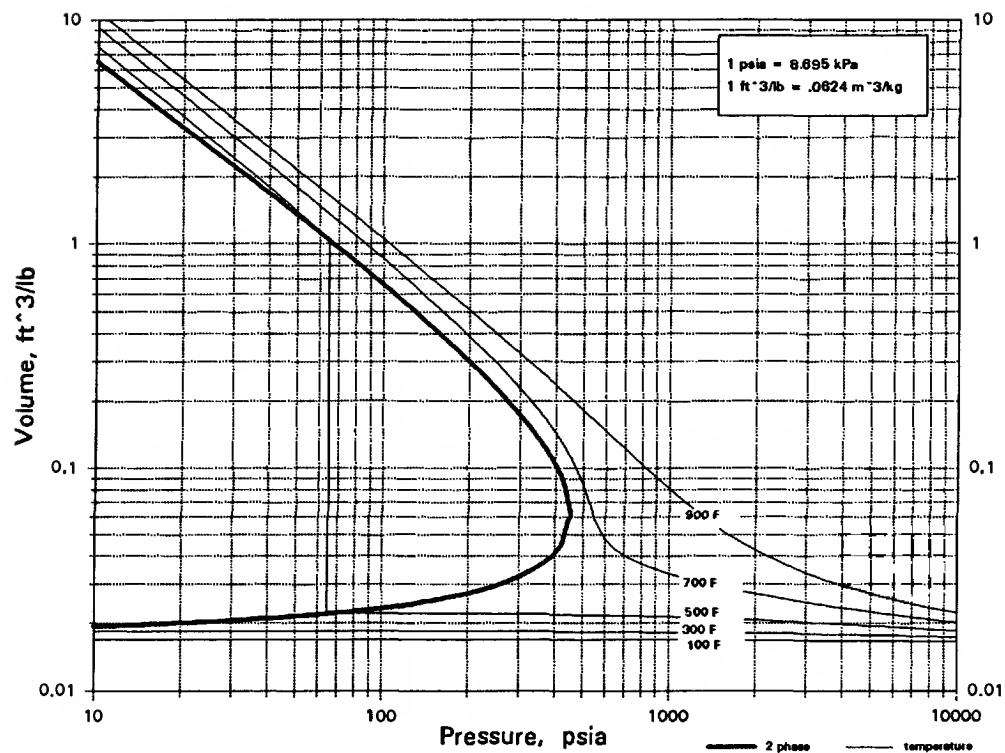


C6H14O3
DIPROPYLENE GLYCOL



C6H14O3

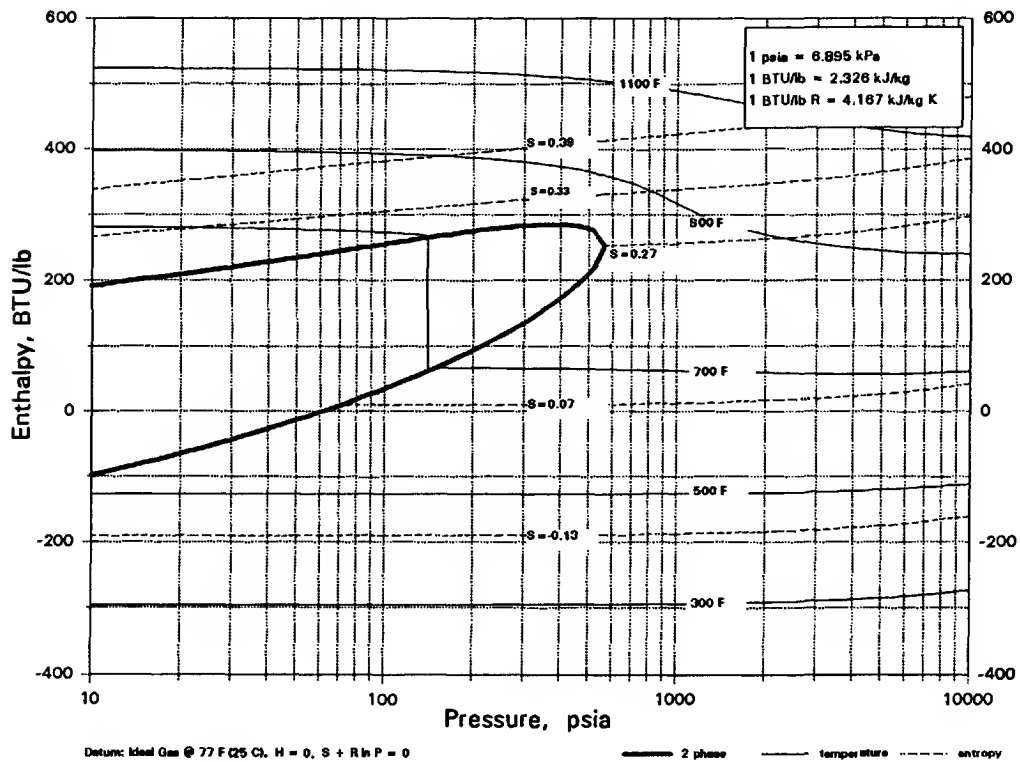
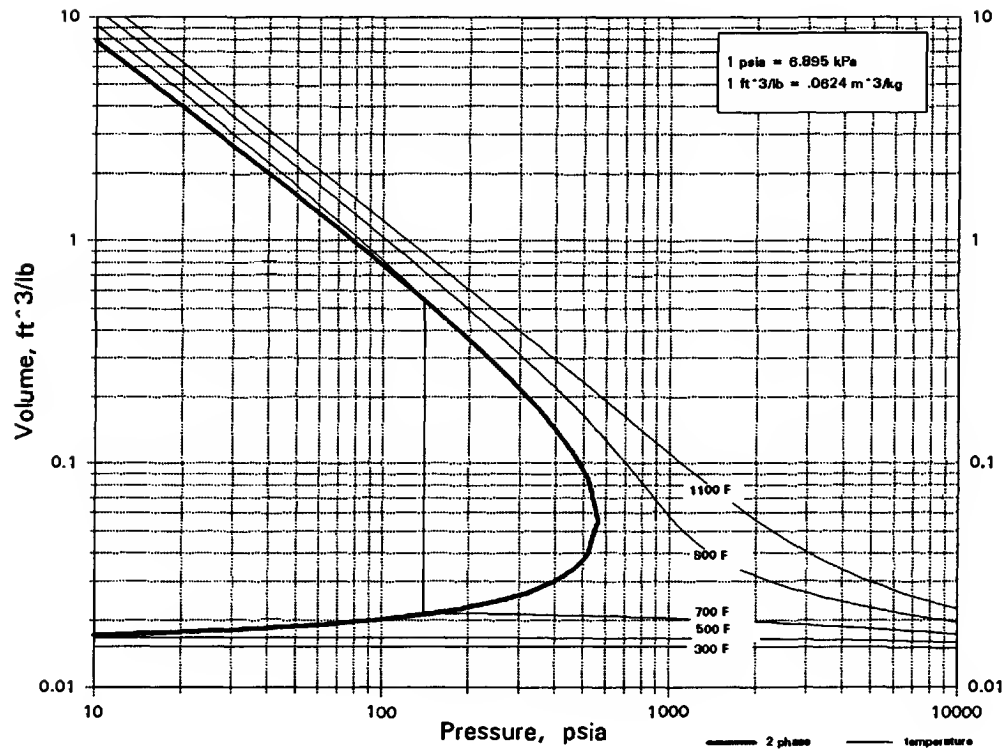
2-(2-ETHOXYETHOXY)ETHANOL



Reference Ideal Gas @ 77 F (25 C): $H = 0$, $S + R \ln P = 0$

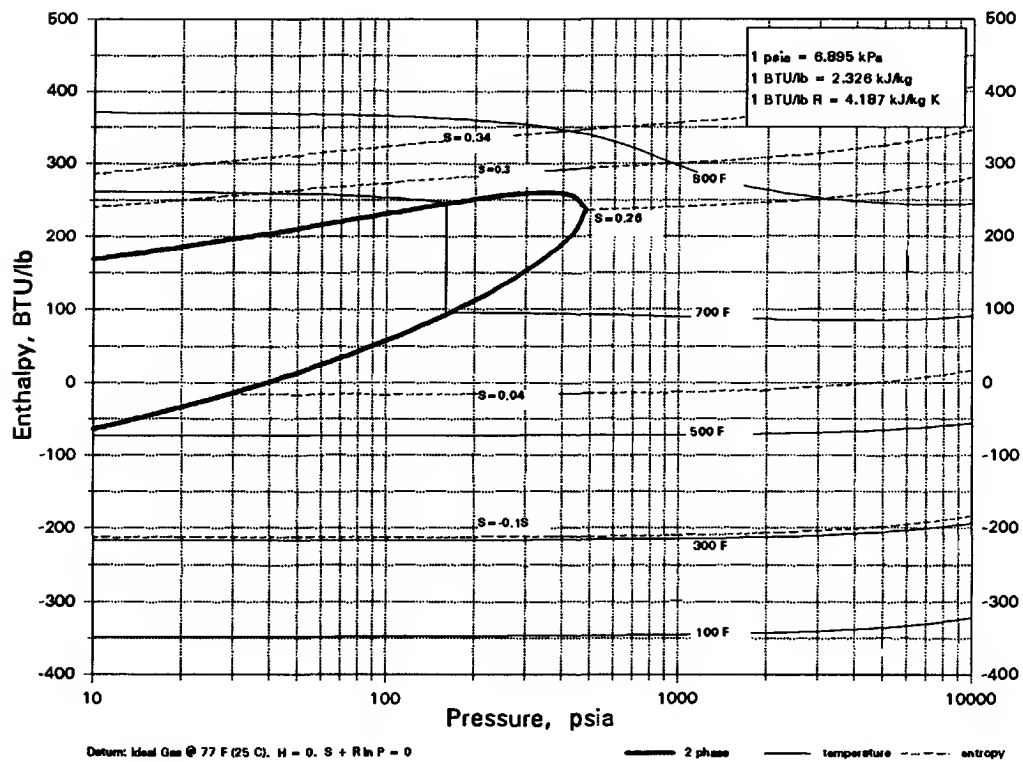
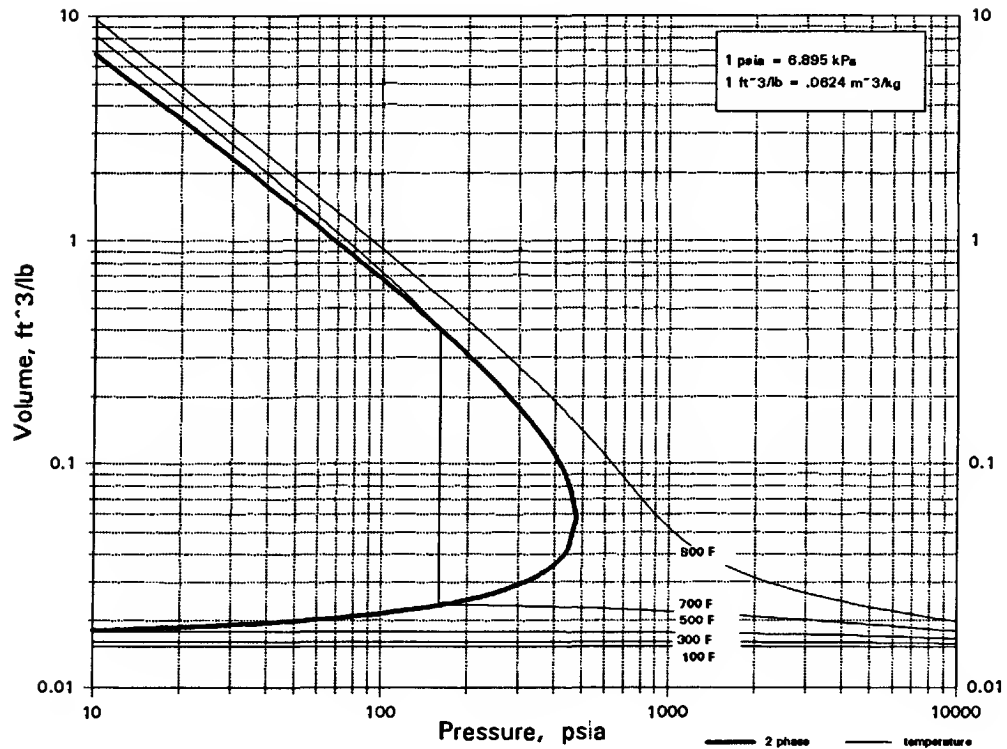
C6H14O3

TRIMETHYLOLPROPANE



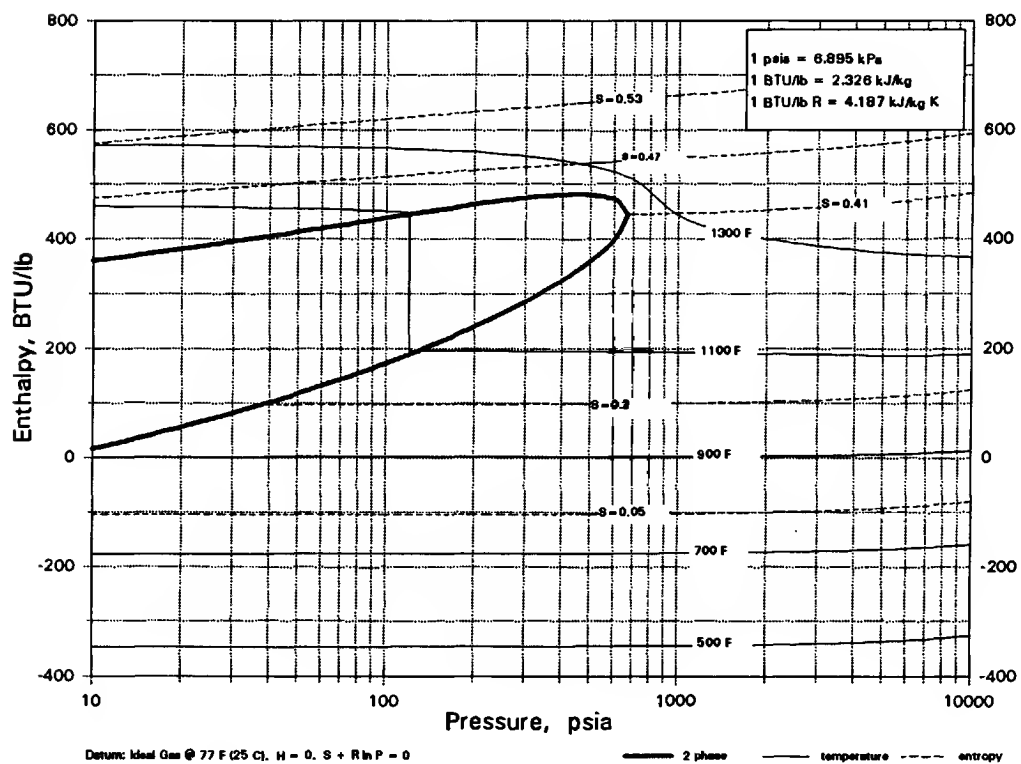
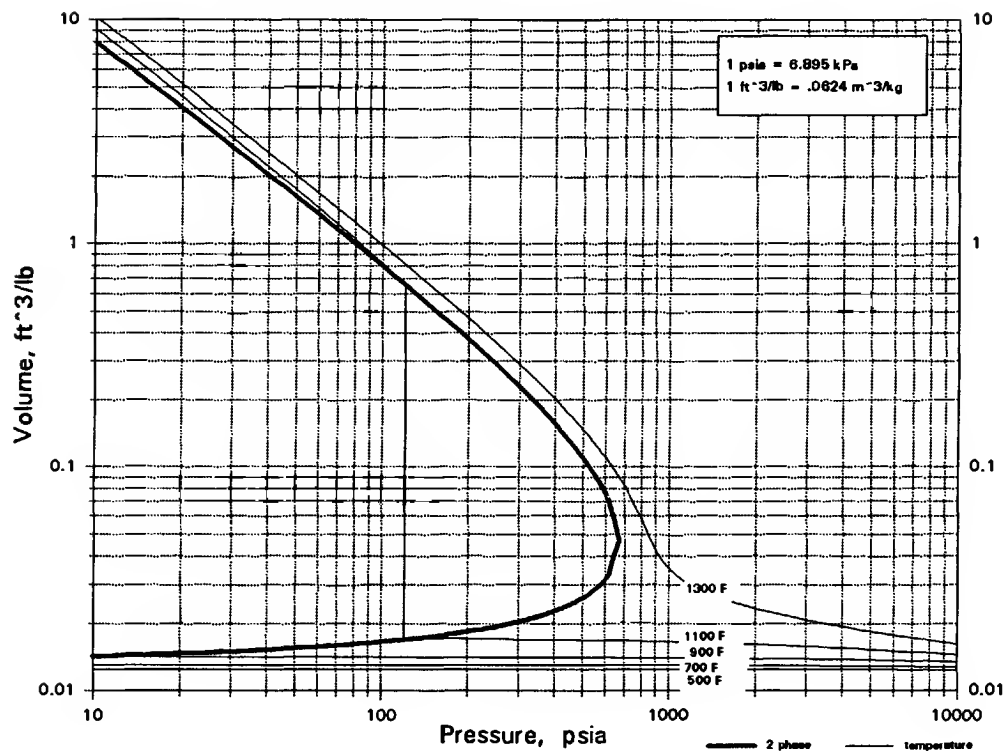
C6H14O4

TRIETHYLENE GLYCOL



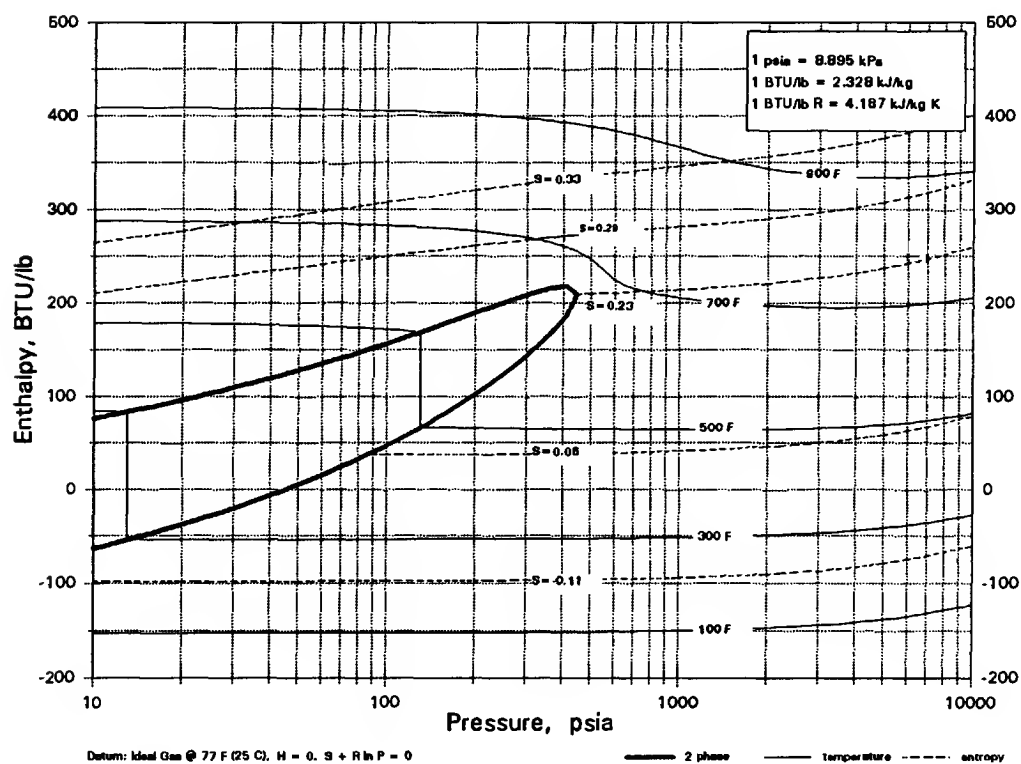
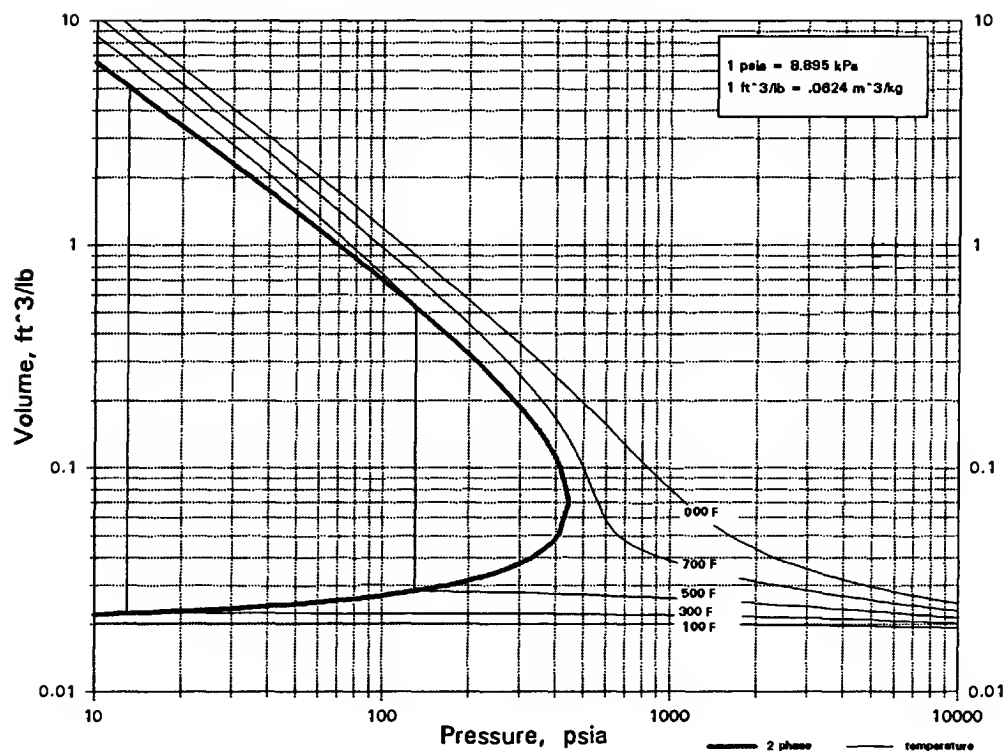
C6H14O6

SORBITOL



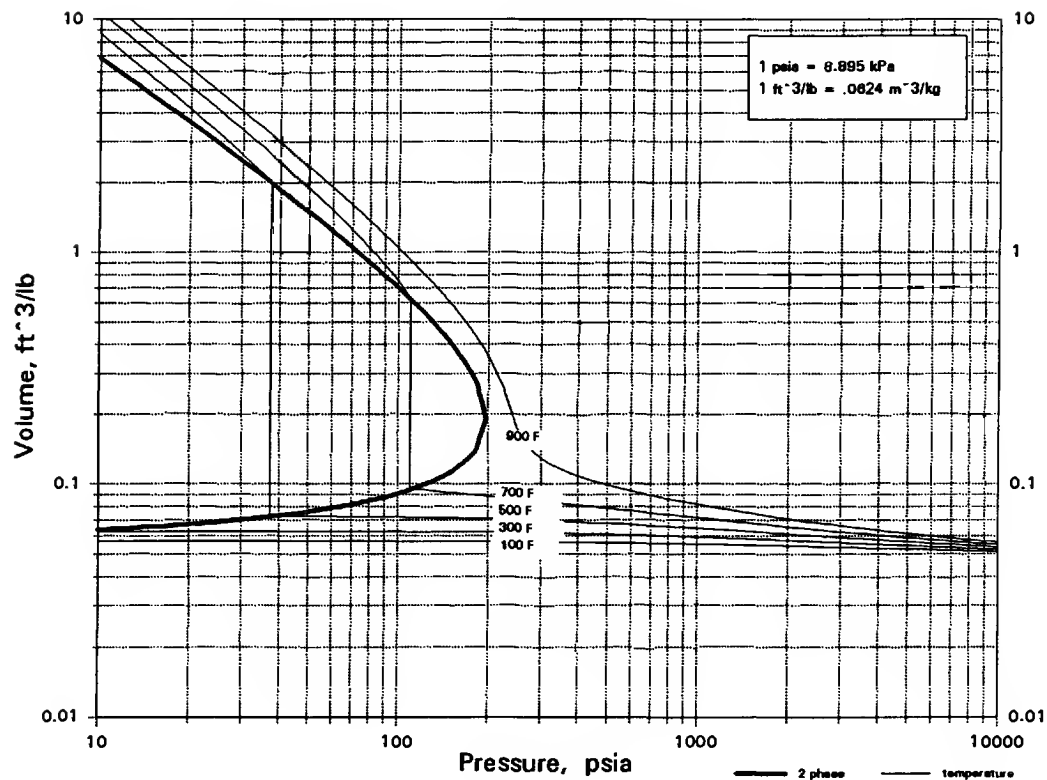
C6H14S

n-HEXYLMERCAPTAN



C6H15Al

TRIETHYL ALUMINIUM



1. Boiling Point, K..... 458.15

2. Critical Temperature, K.... 720.15

3. Critical Pressure, atm..... 13.40

Heat capacity data are not available.

C₆H₁₅Al₂Cl₃	ETHYL ALUMINUM SESQUICHLORIDE
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1. Molecular Weight, lb/mol..... 247.51

2. Boiling Point, K..... 482.15

Critical data (T_c, P_c) are not available.

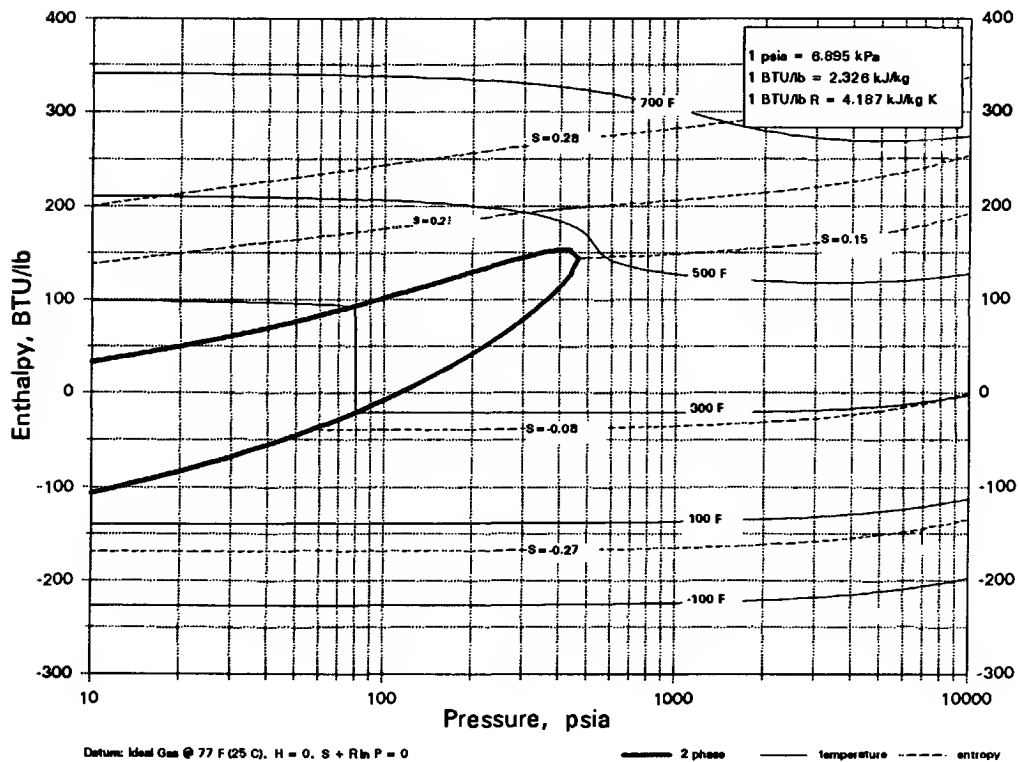
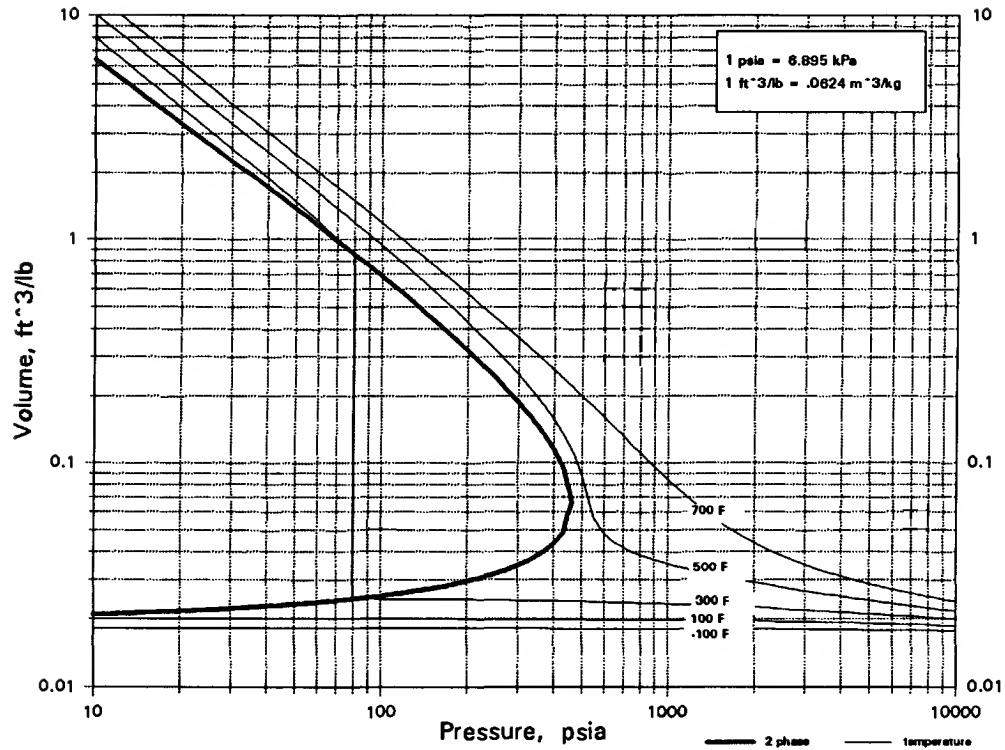
1. Molecular Weight, lb/mol..... 247.51

2. Boiling Point, K..... 482.15

Critical data (T_c, P_c) are not available.

C6H15N

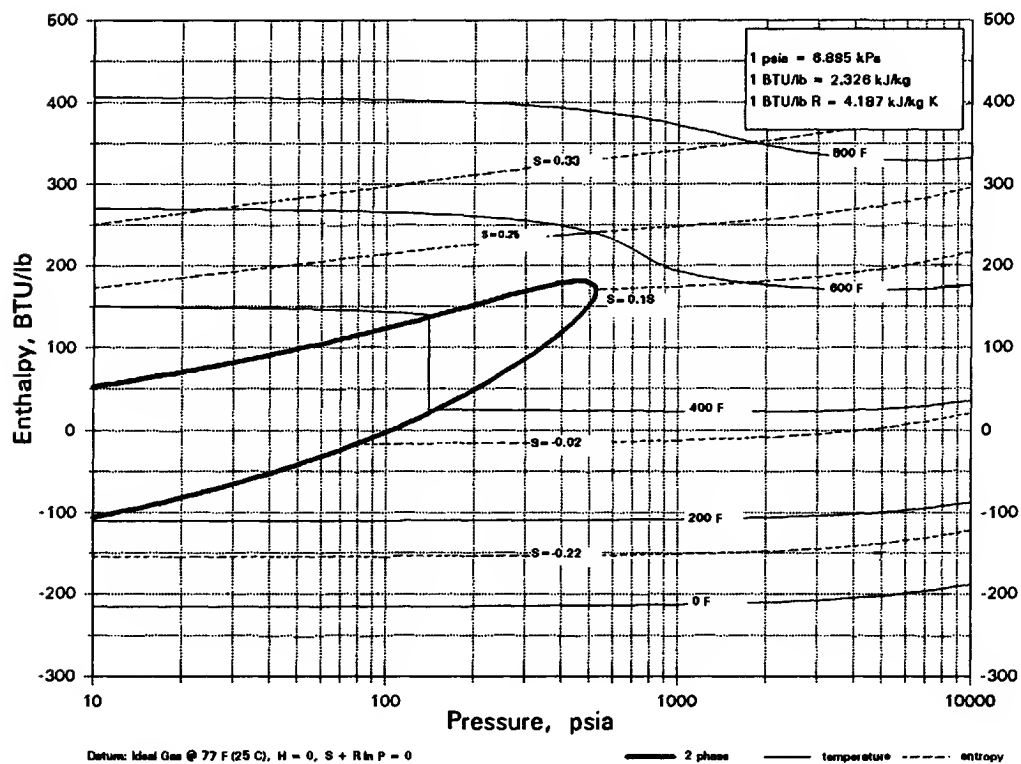
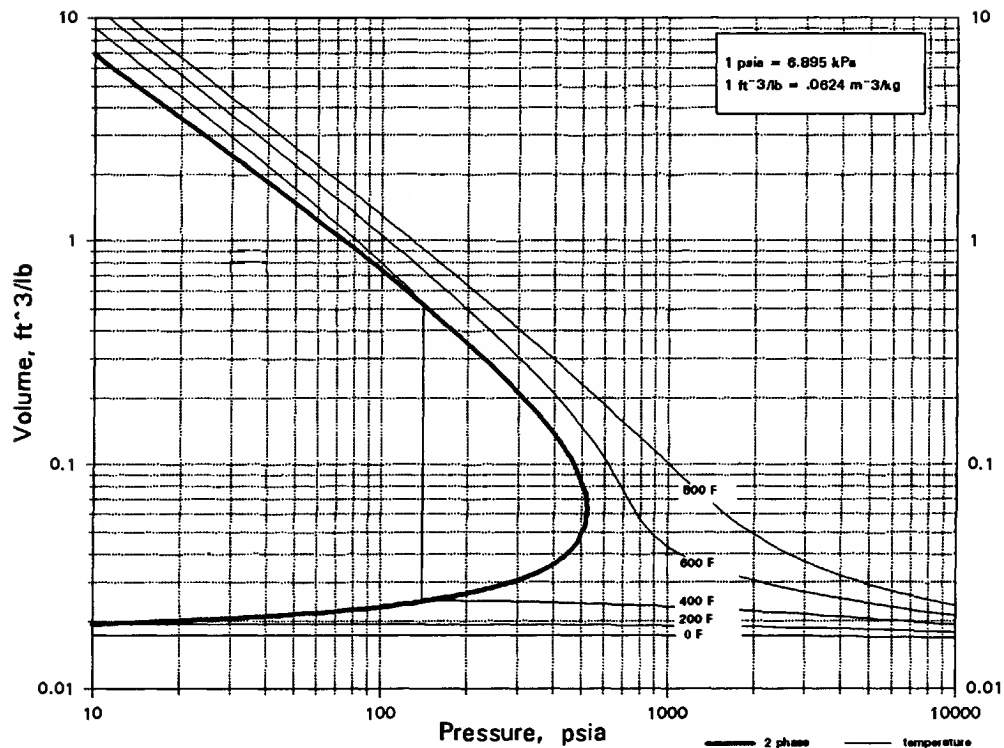
DIISOPROPYLAMINE



Devote: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

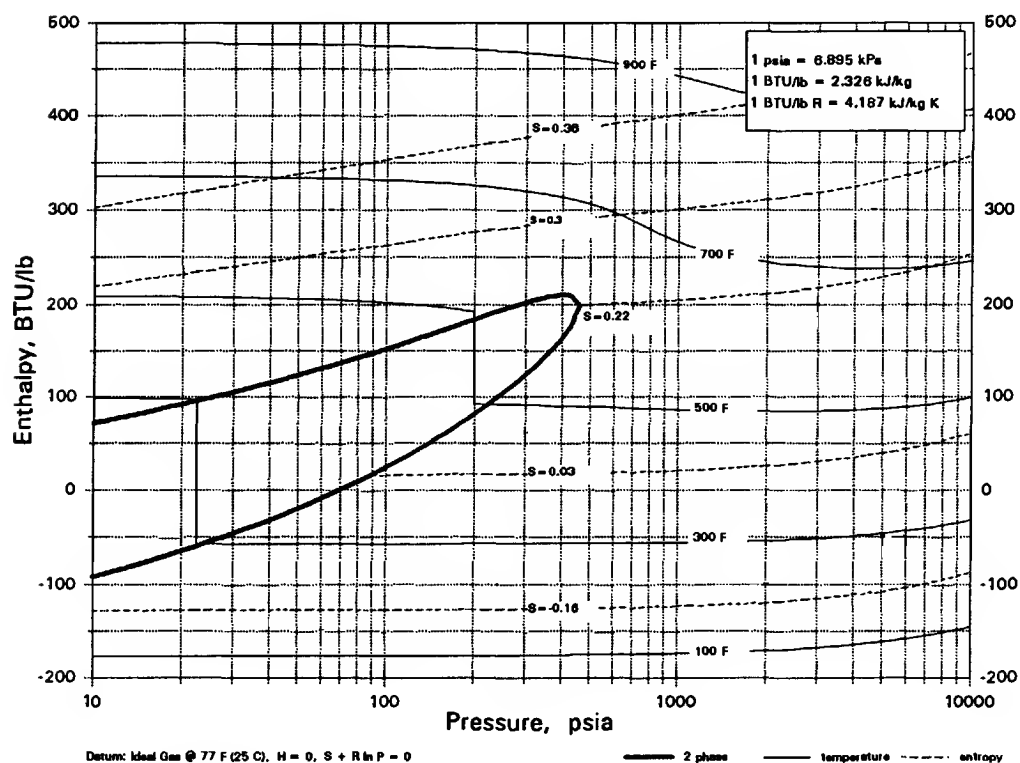
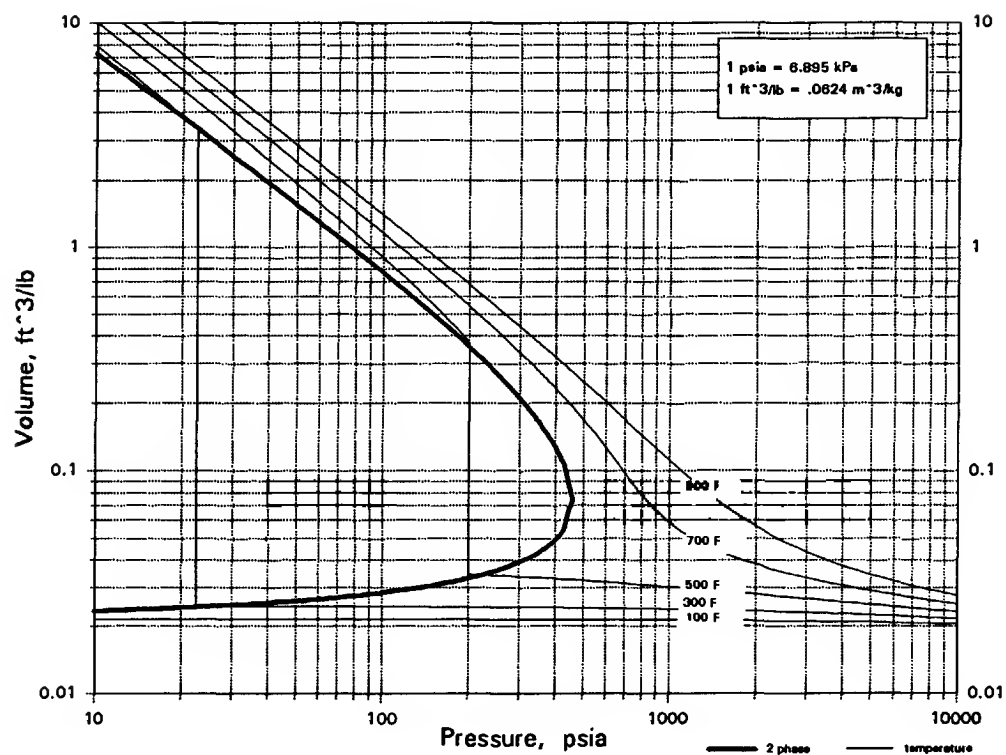
C6H15N

DI-n-PROPYLAMINE

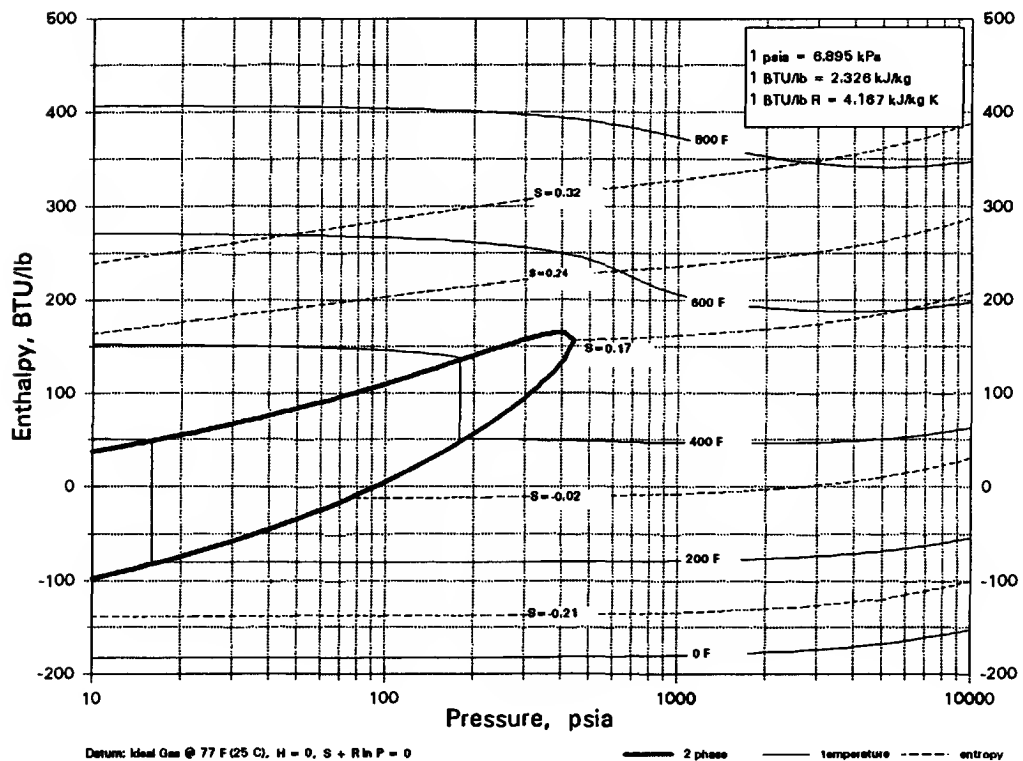
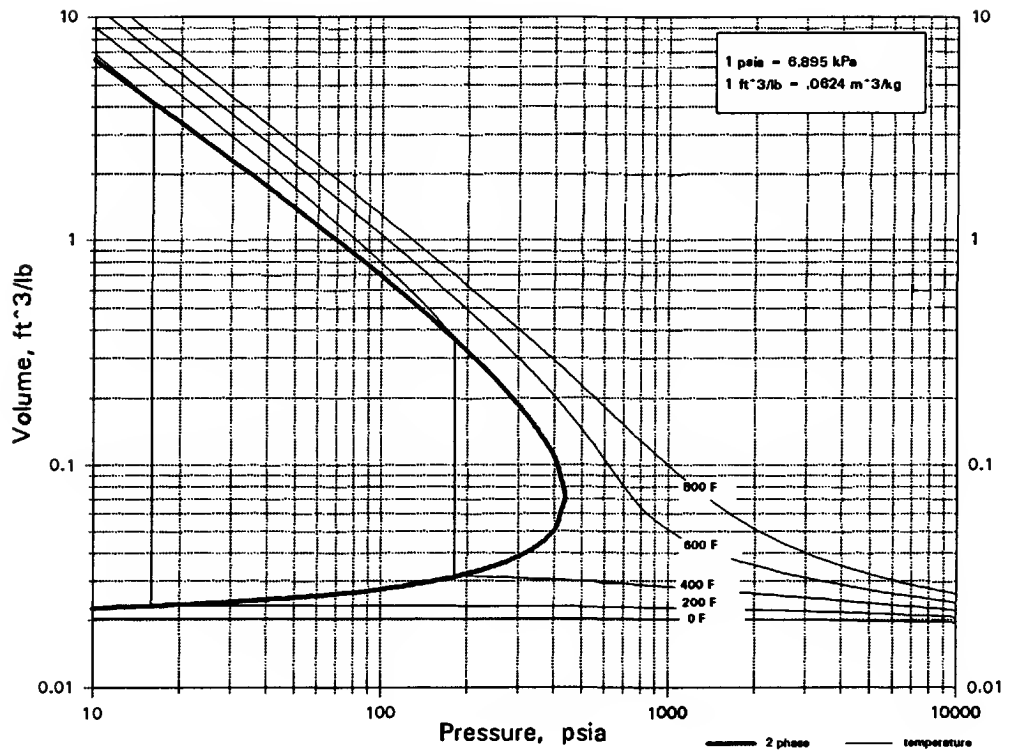


C6H15N

n-HEXYLAMINE

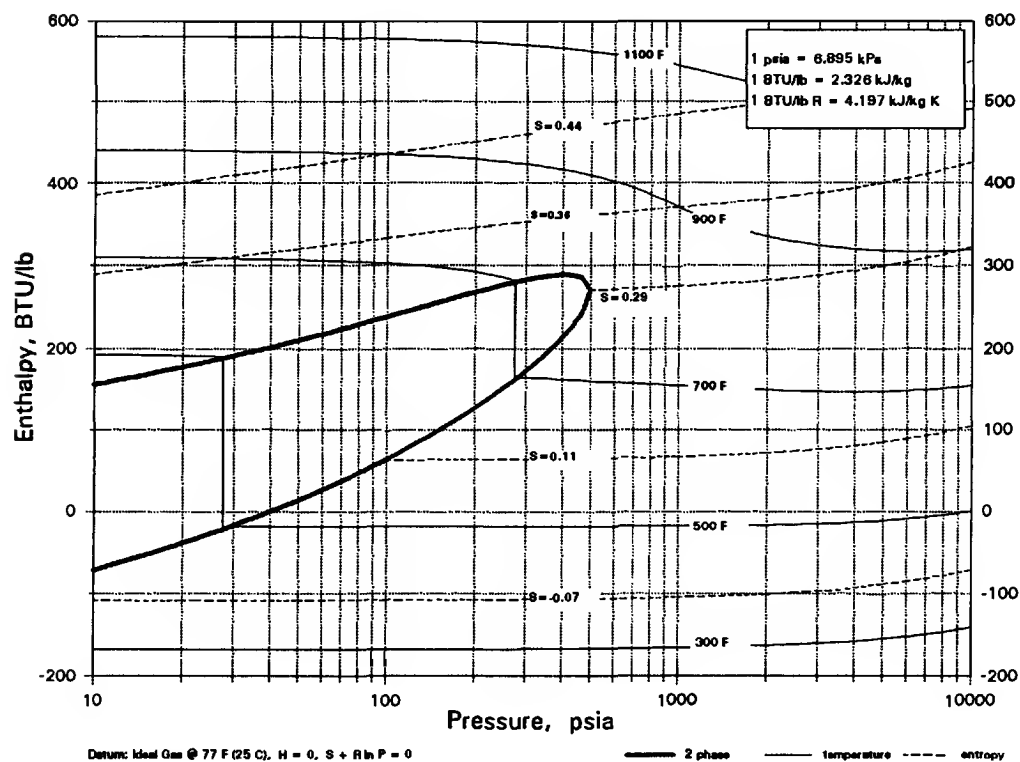
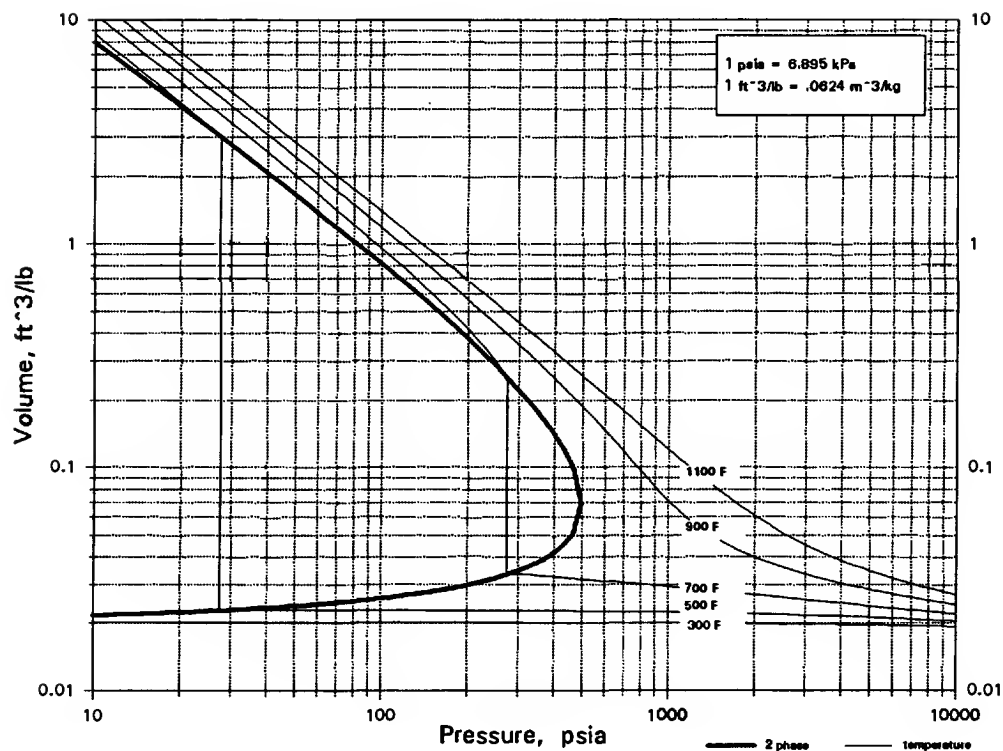


C6H15N
TRIETHYLAMINE



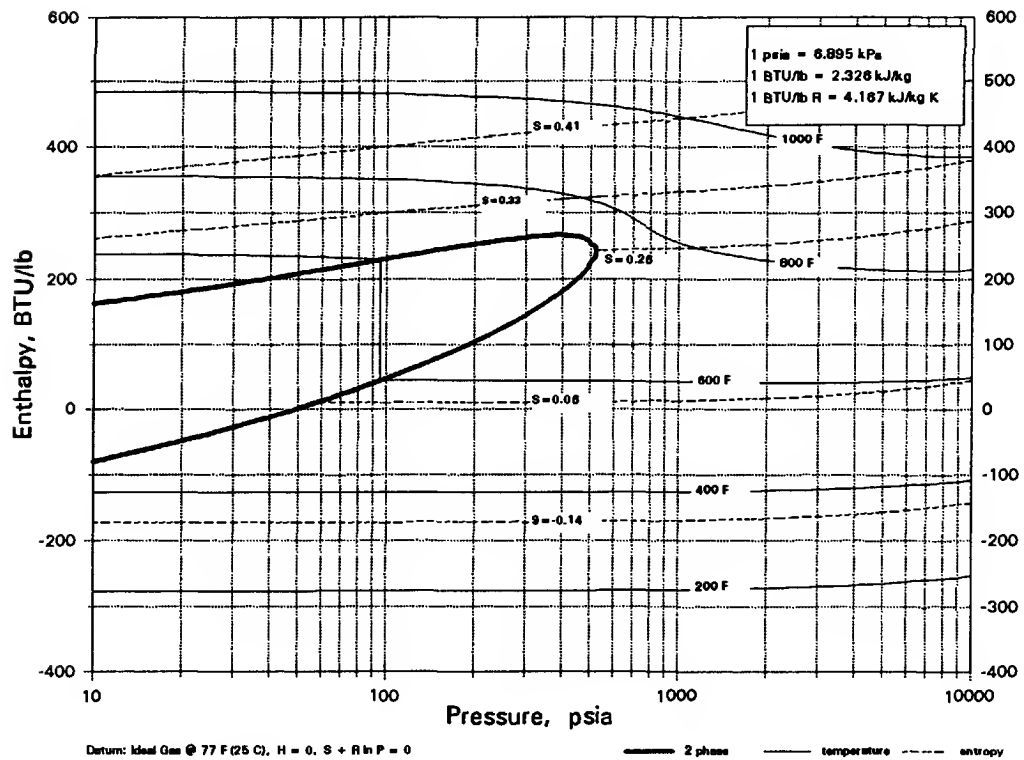
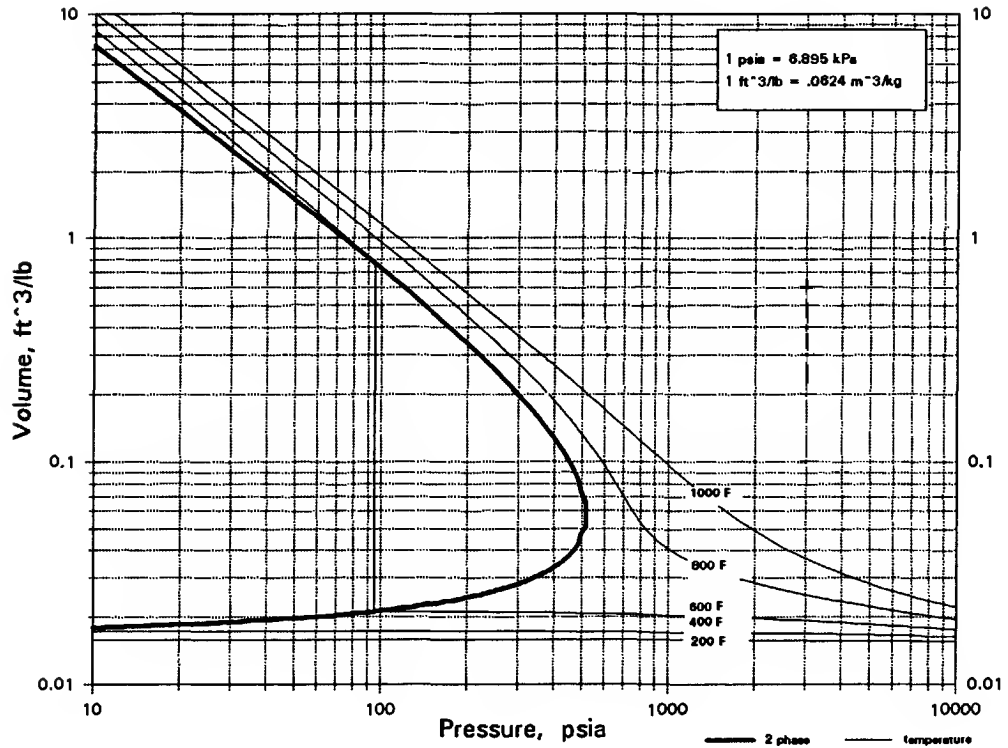
C6H15NO

6-AMINOHEXANOL



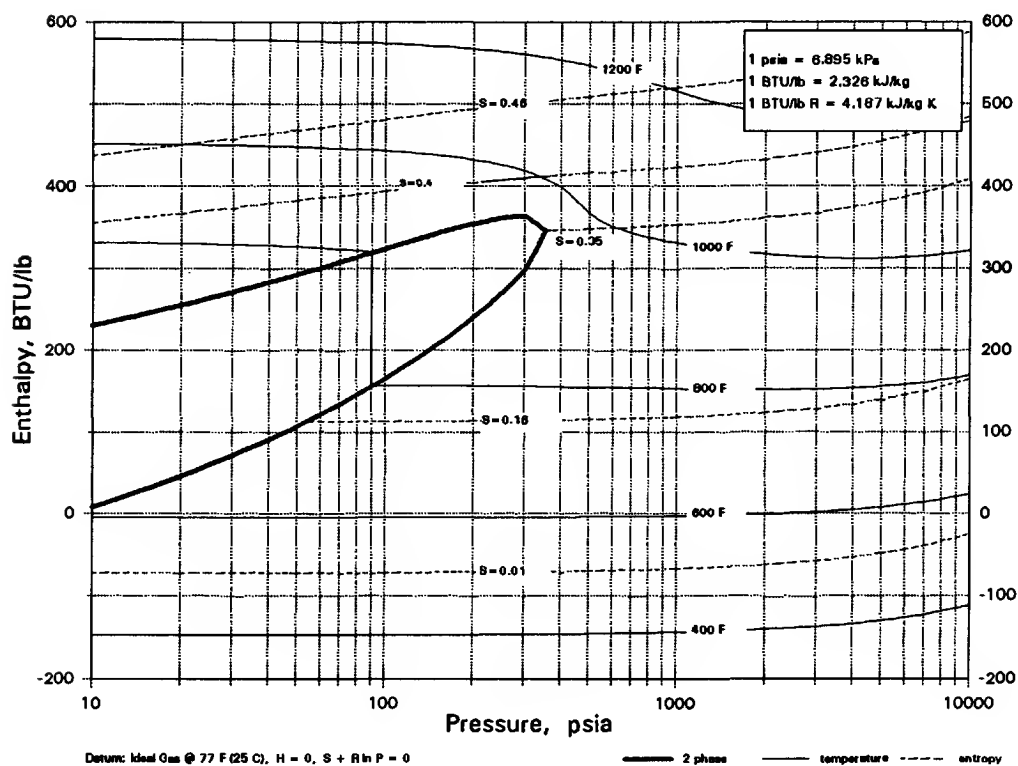
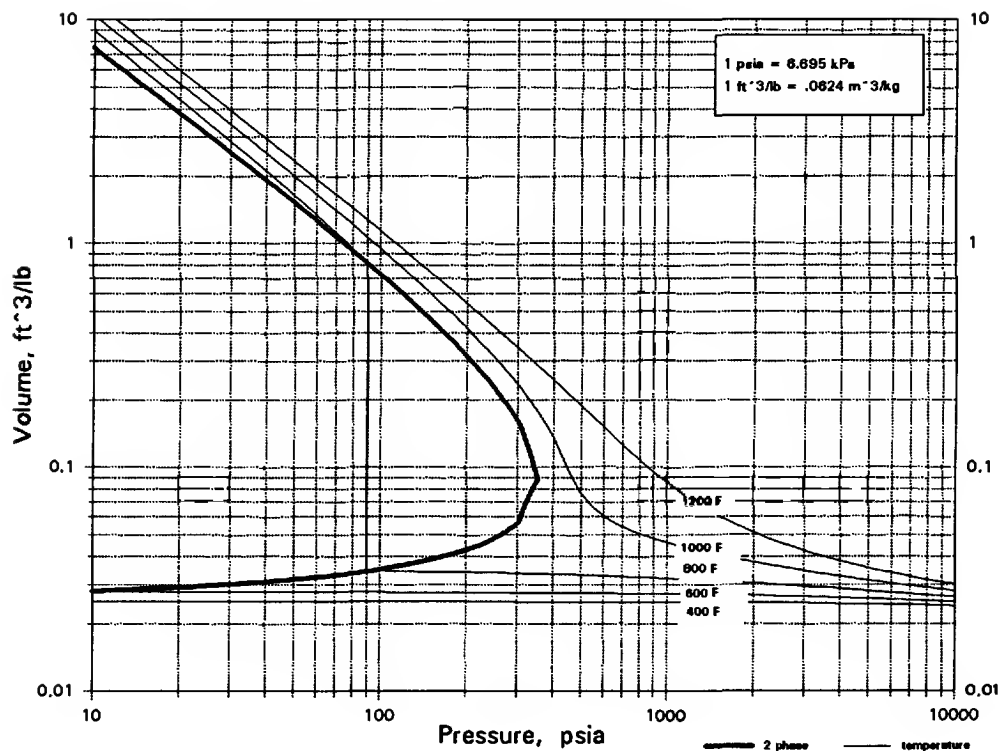
C6H15NO2

DIISOPROPANOLAMINE



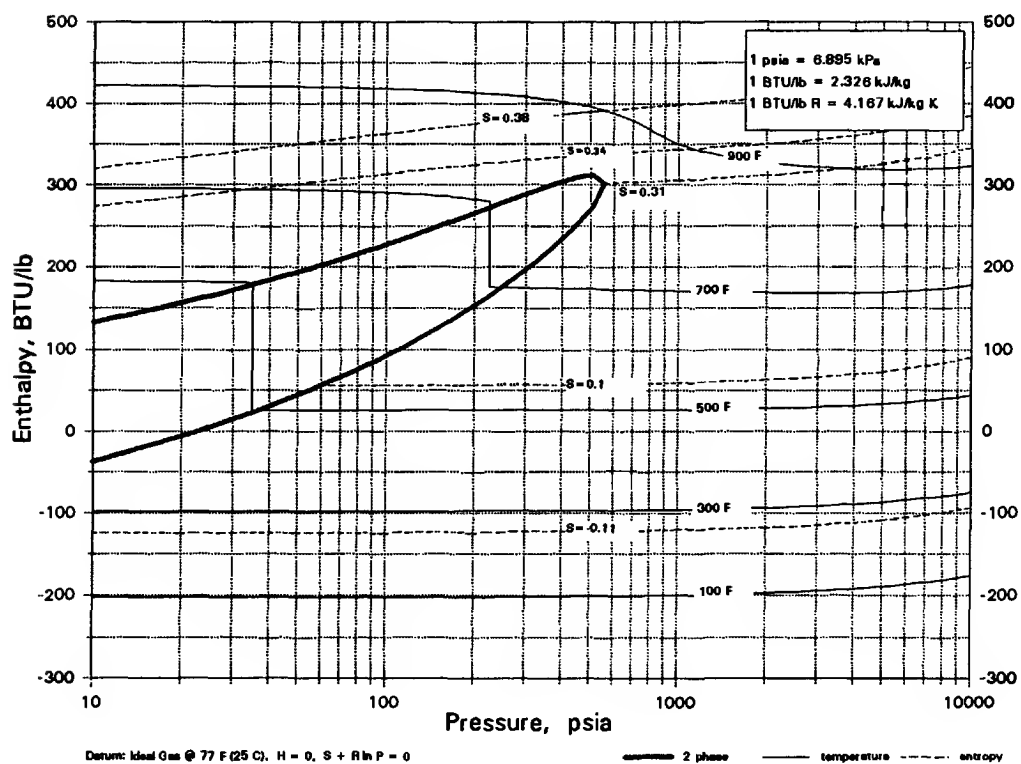
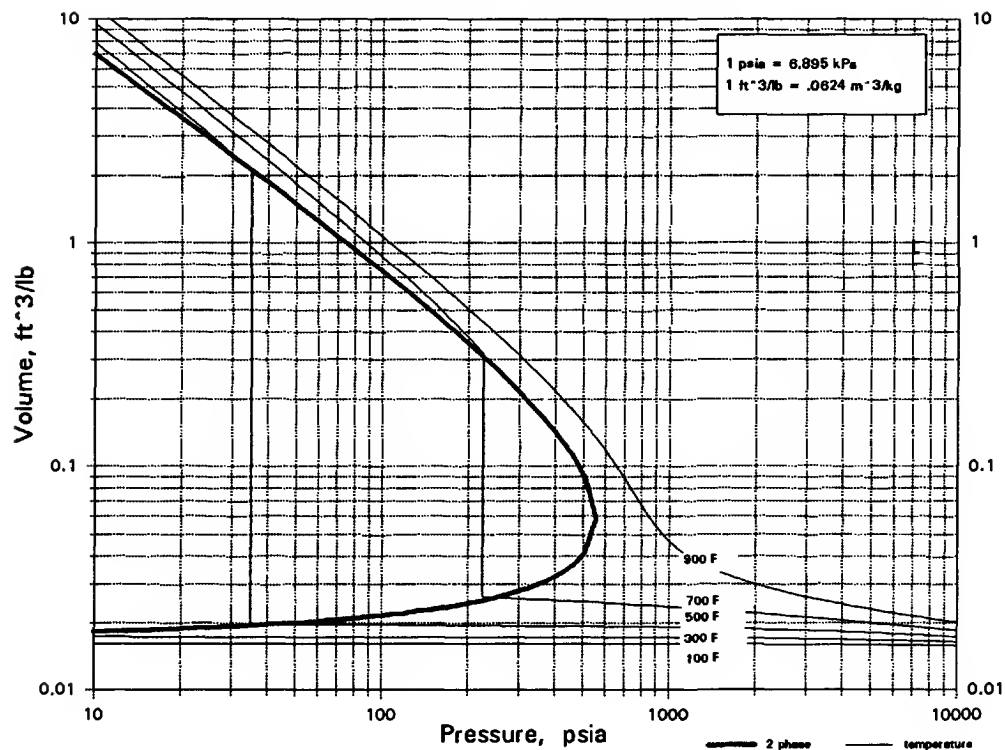
C6H15NO3

TRIETHANOLAMINE



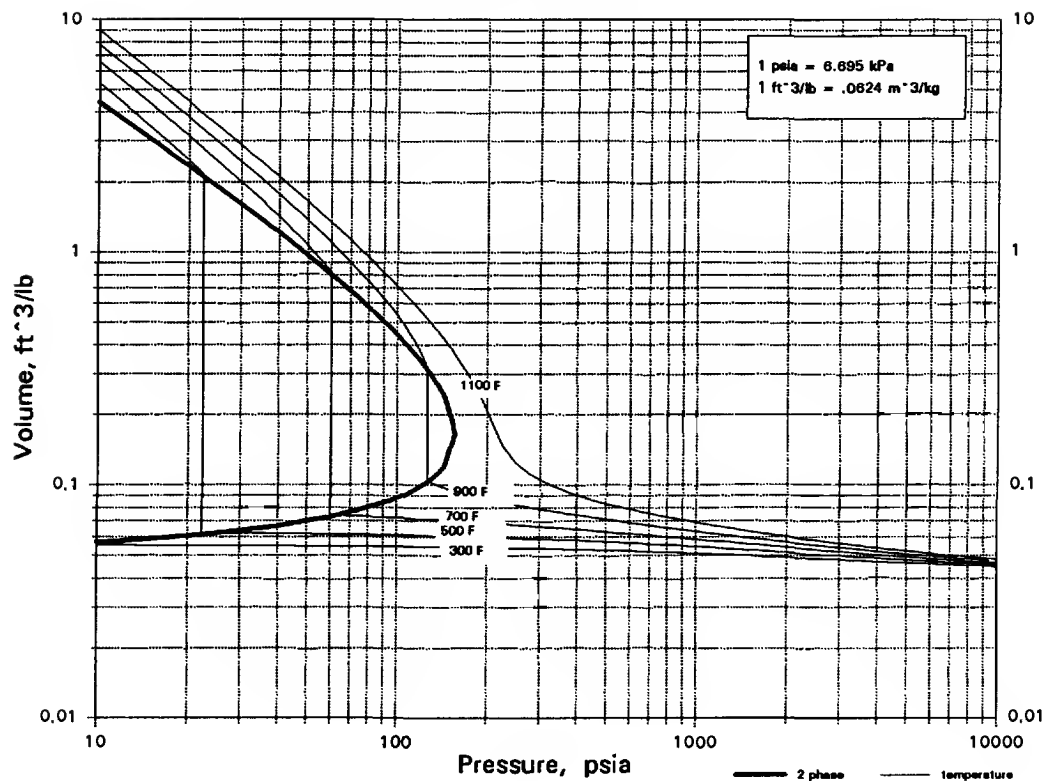
C6H15N3

N-AMINOETHYL PIPERAZINE



C6H15O4P

TRIETHYL PHOSPHATE



1. Boiling Point, K..... 484.15

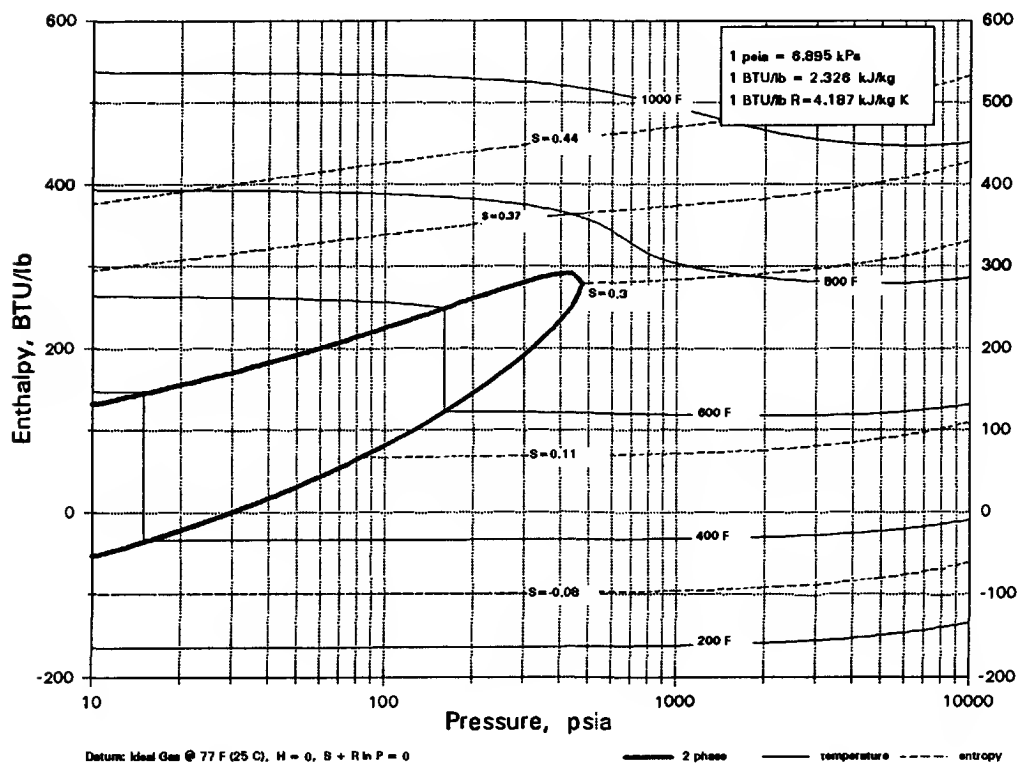
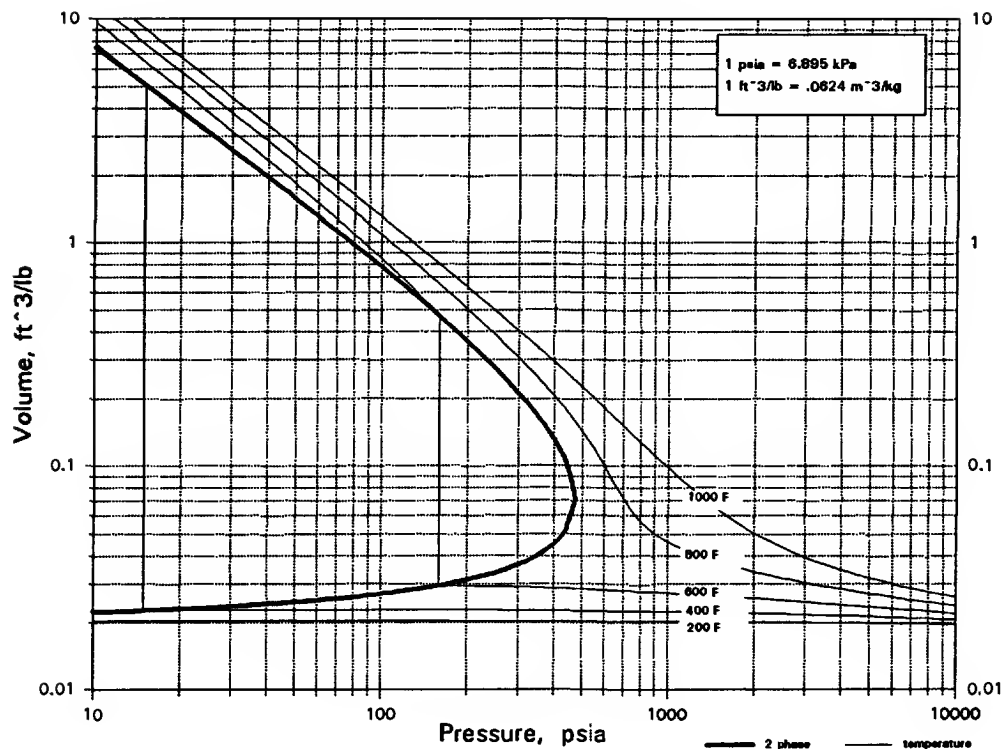
2. Critical Temperature, K.... 794.00

3. Critical Pressure, atm..... 10.66

Heat capacity data are not available.

C6H16N2

HEXAMETHYLENEDIAMINE



1. Molecular Weight, lb/mol..... 179.20

2. Boiling Point, K..... 506.15

Critical data (Tc, Pc) are not available.

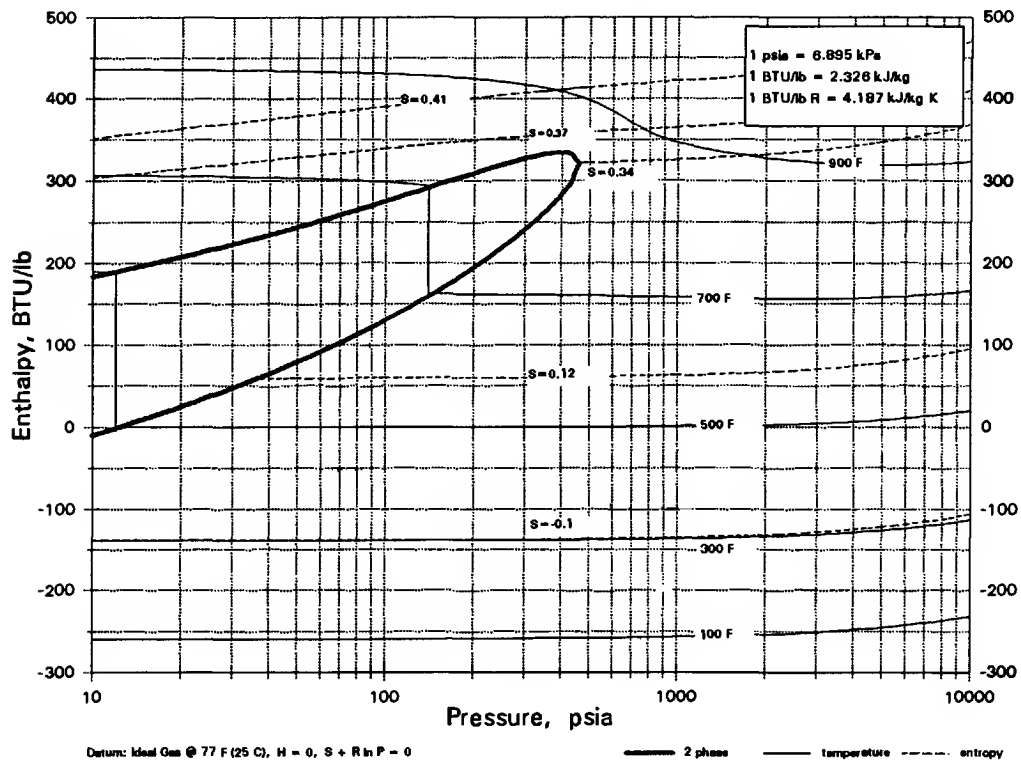
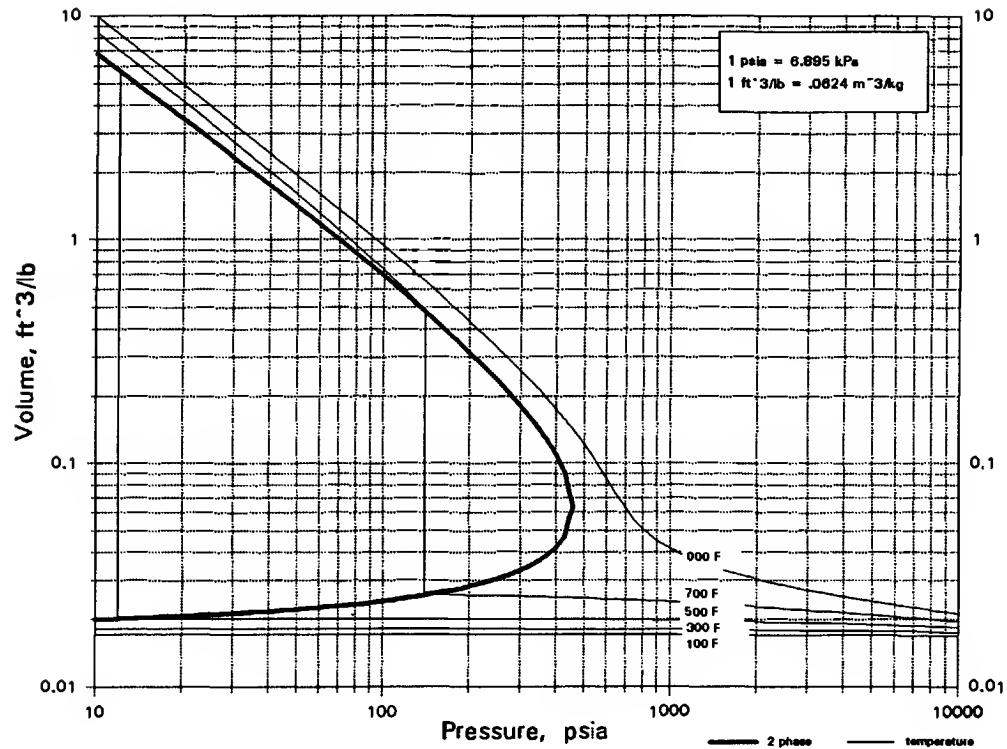
1. Molecular Weight, lb/mol..... 179.20

2. Boiling Point, K..... 506.15

Critical data (Tc, Pc) are not available.

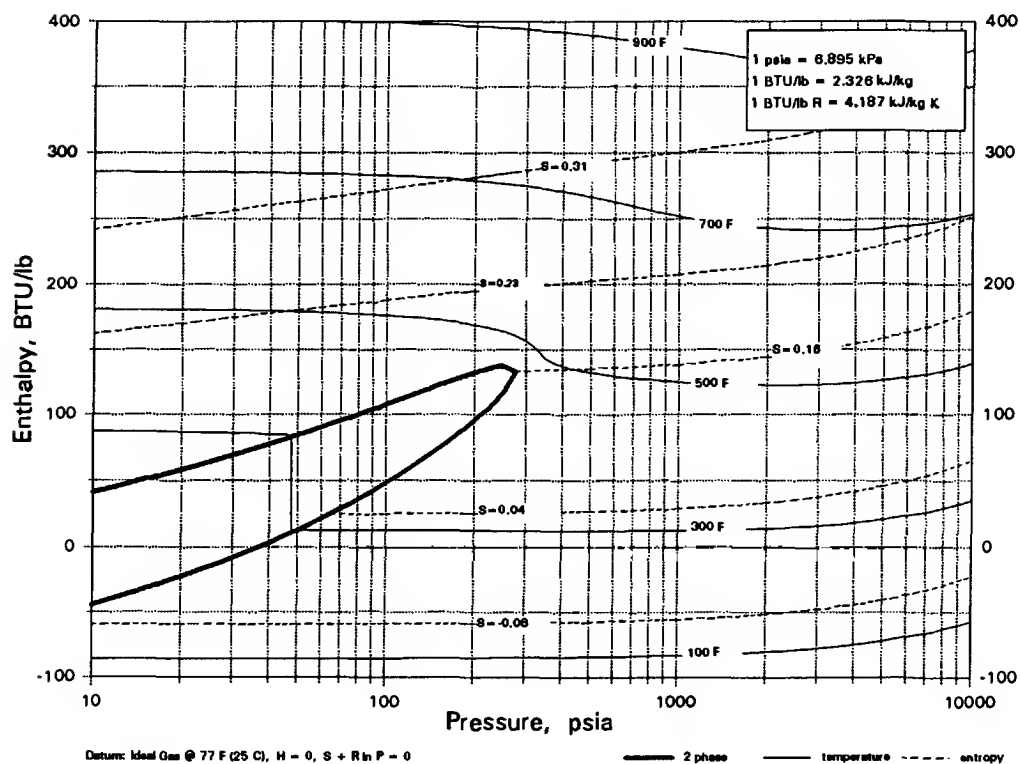
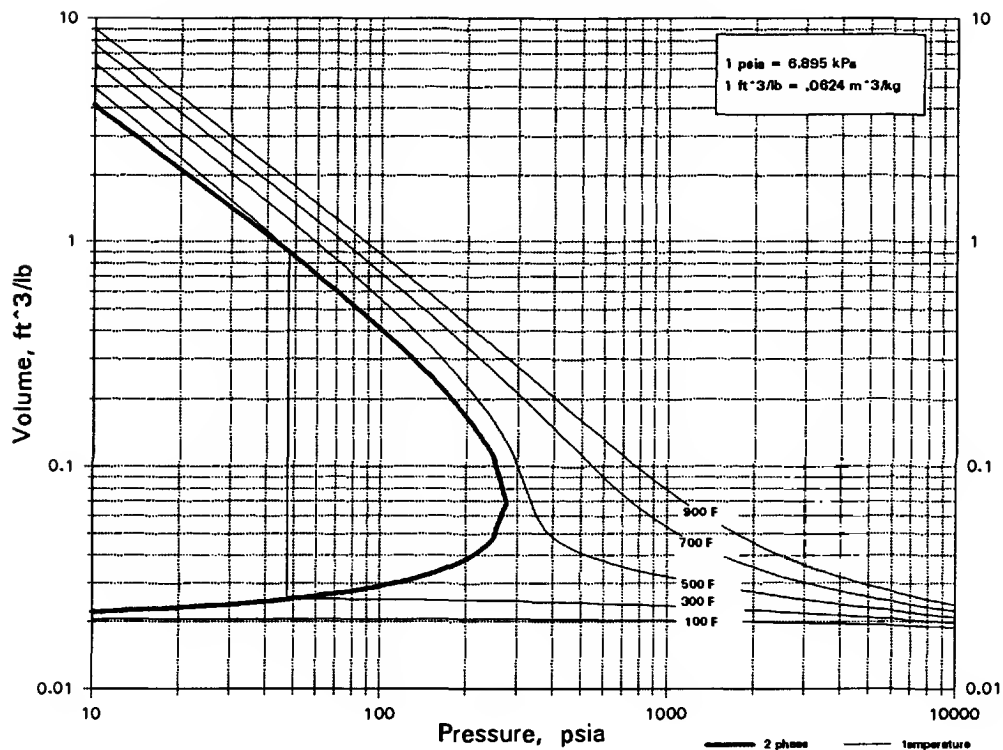
C6H18N4

TRIETHYLENE TETRAMINE

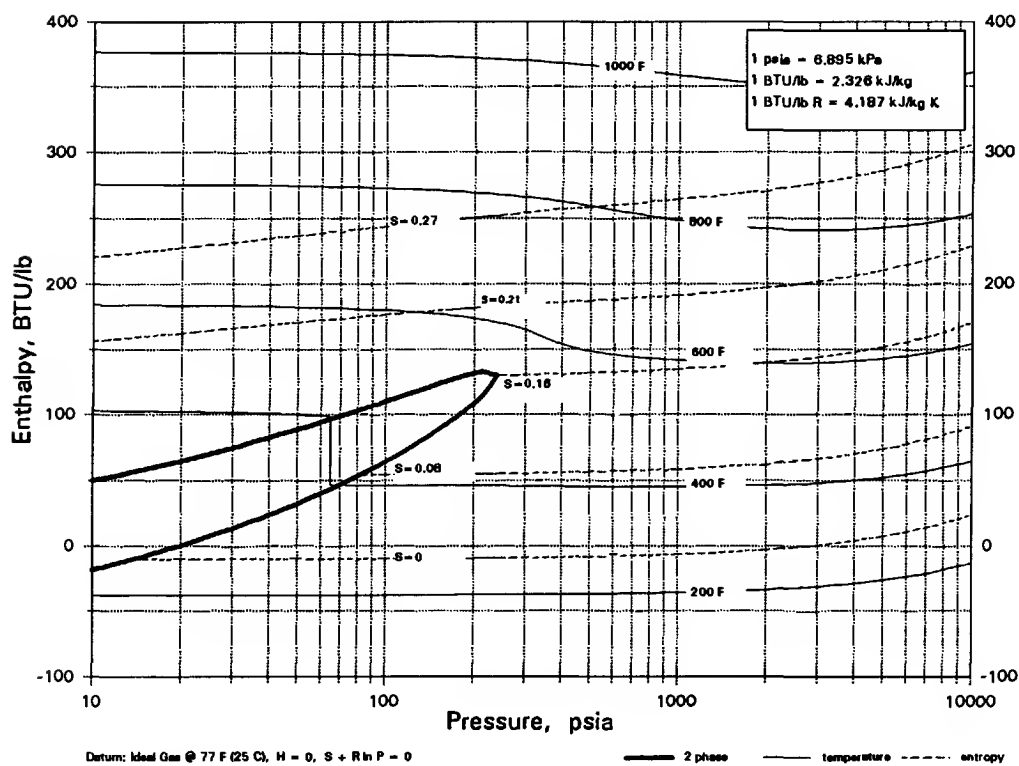
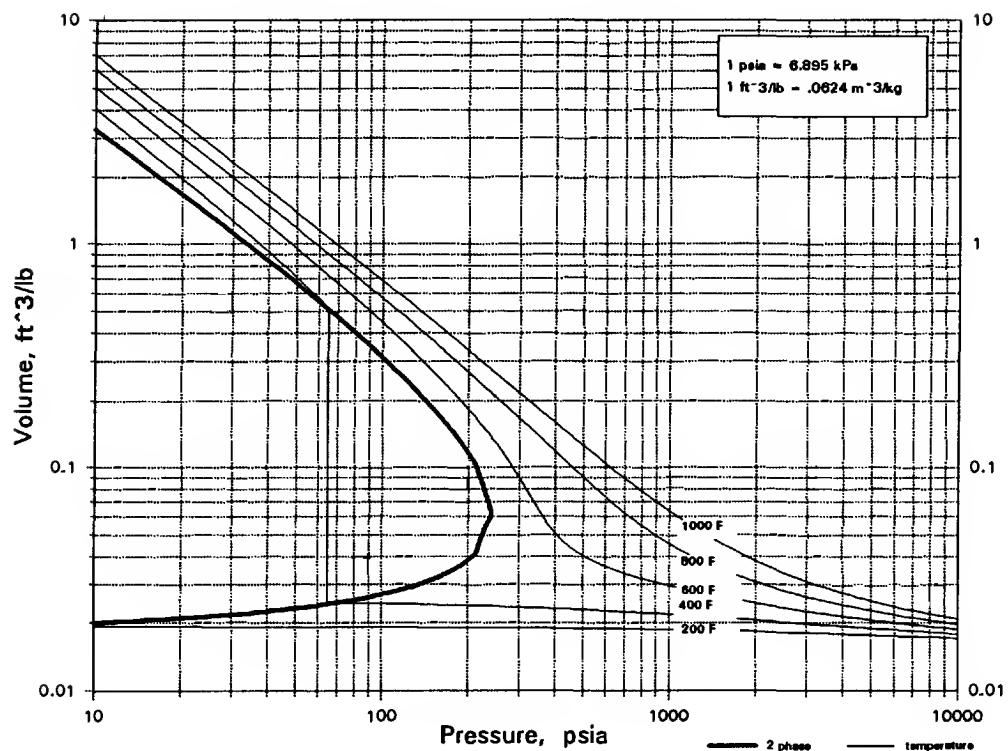


C6H18OSi2

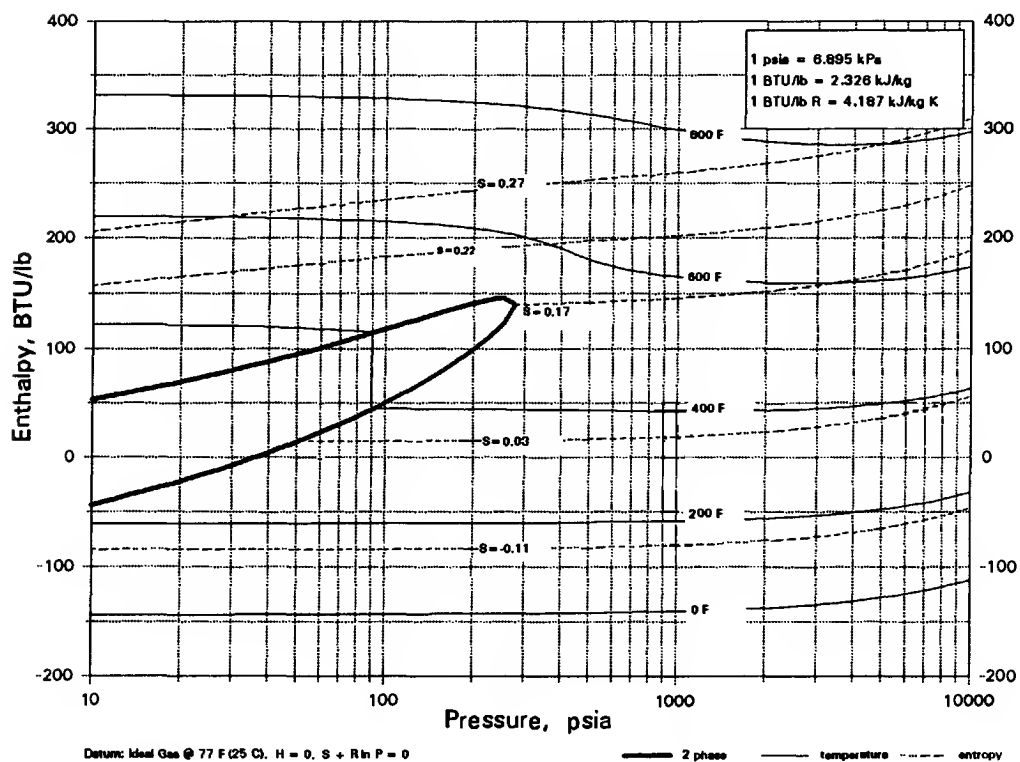
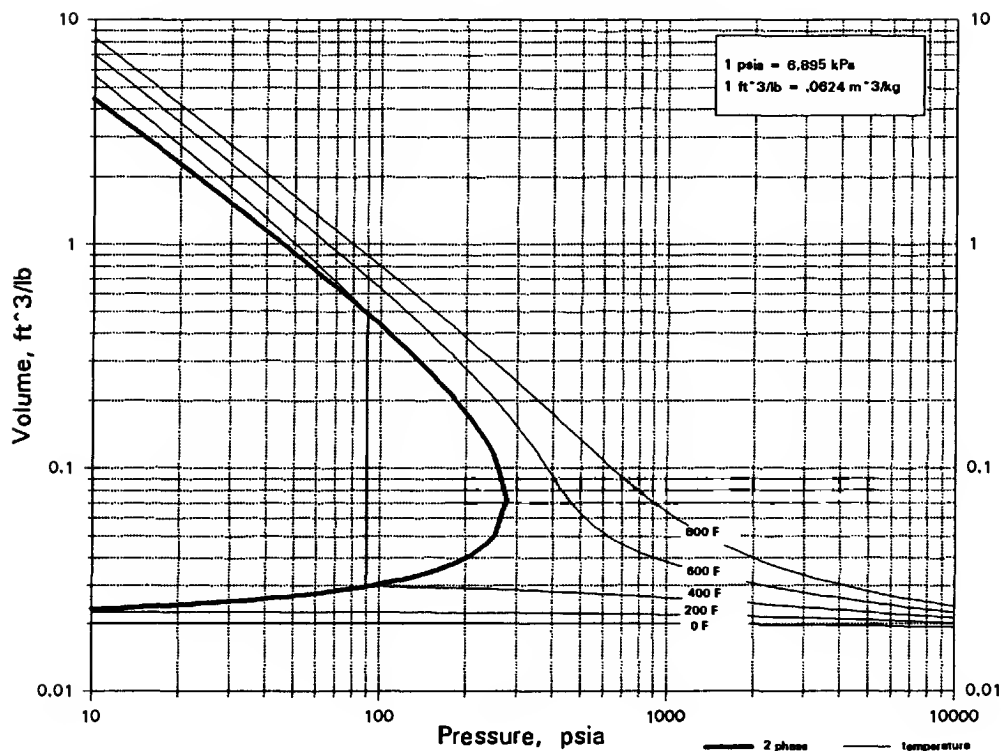
HEXAMETHYLDISILOXANE



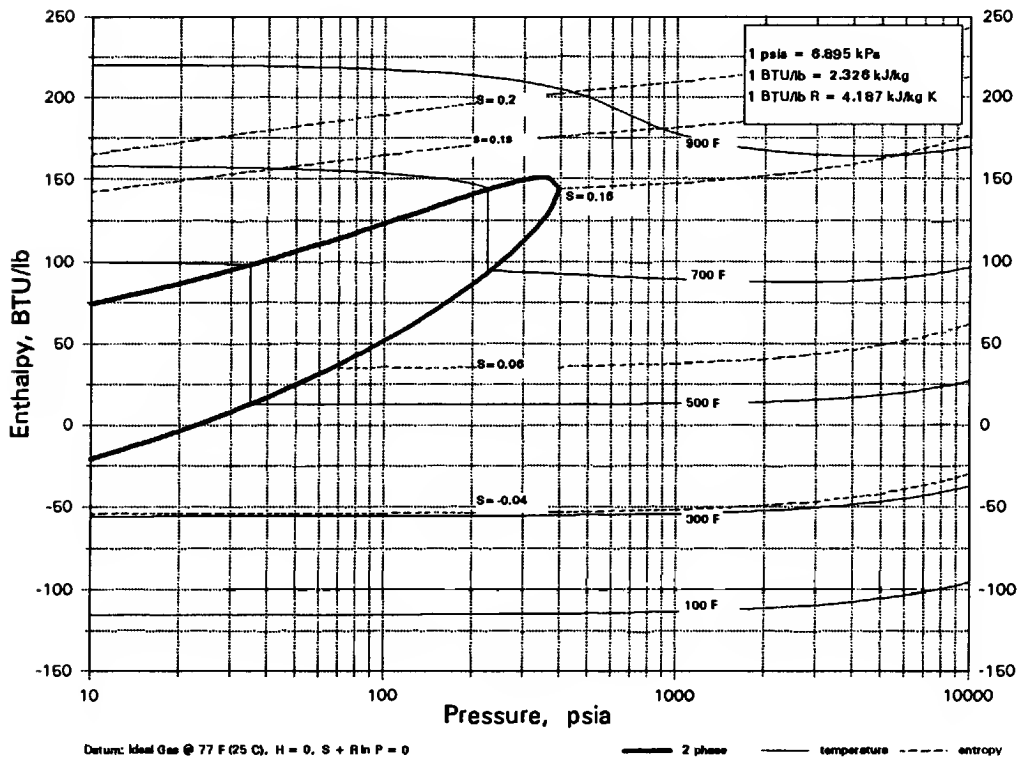
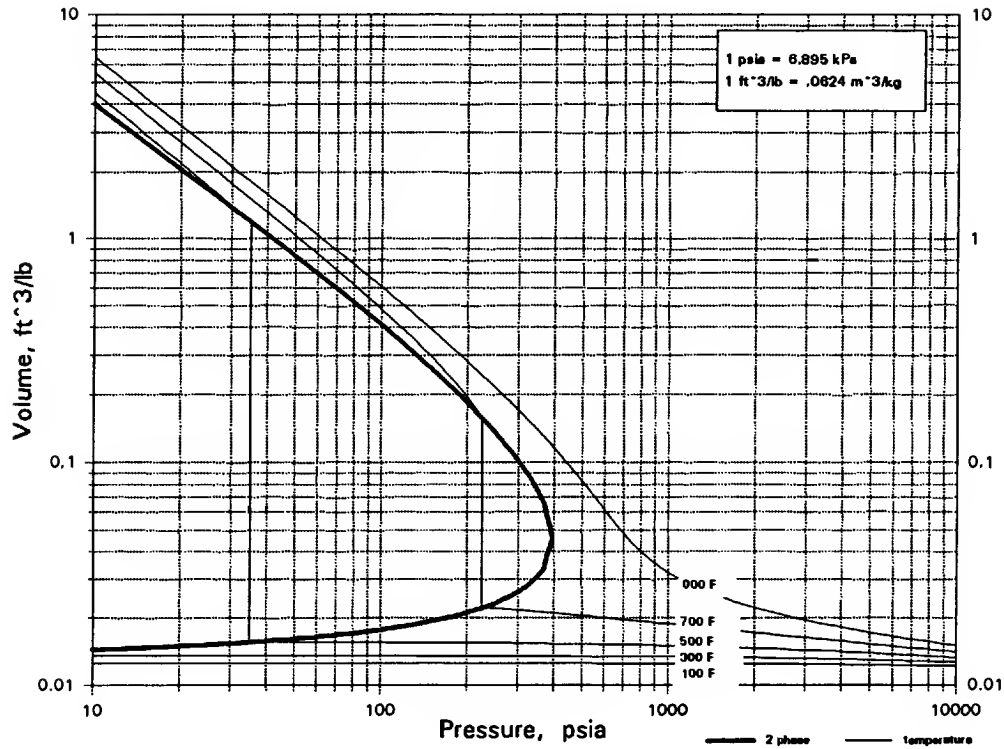
C6H18O3Si3 HEXAMETHYLCYCLOTRISILOXANE



C6H19NSi2 HEXAMETHYLDISILAZANE



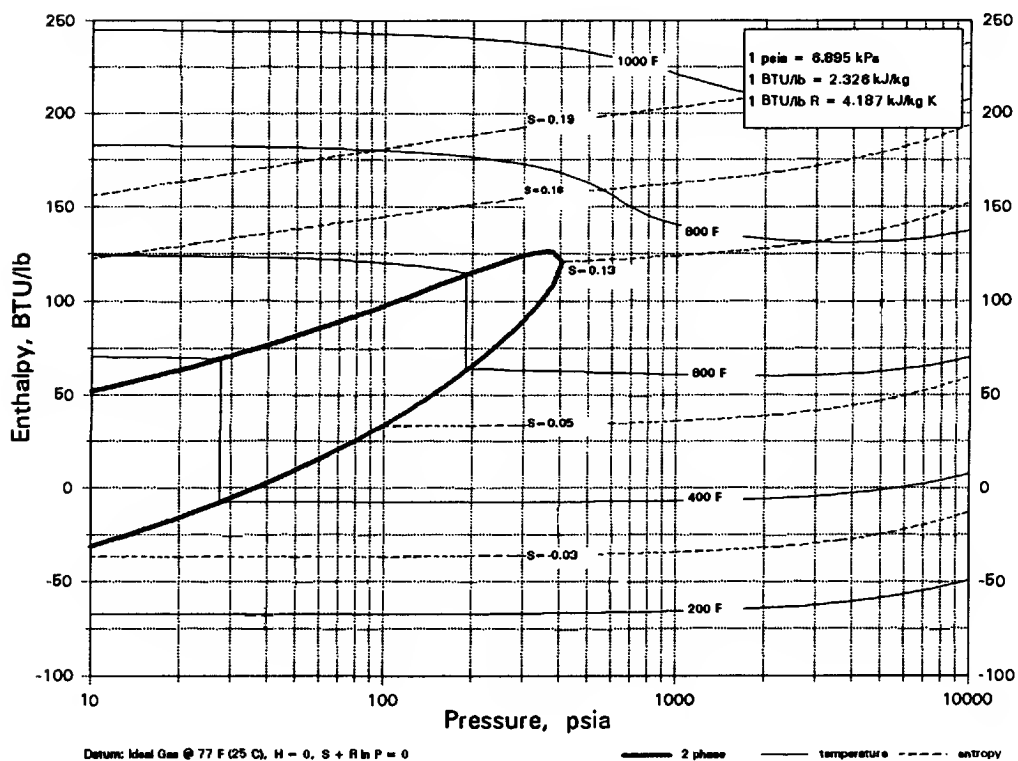
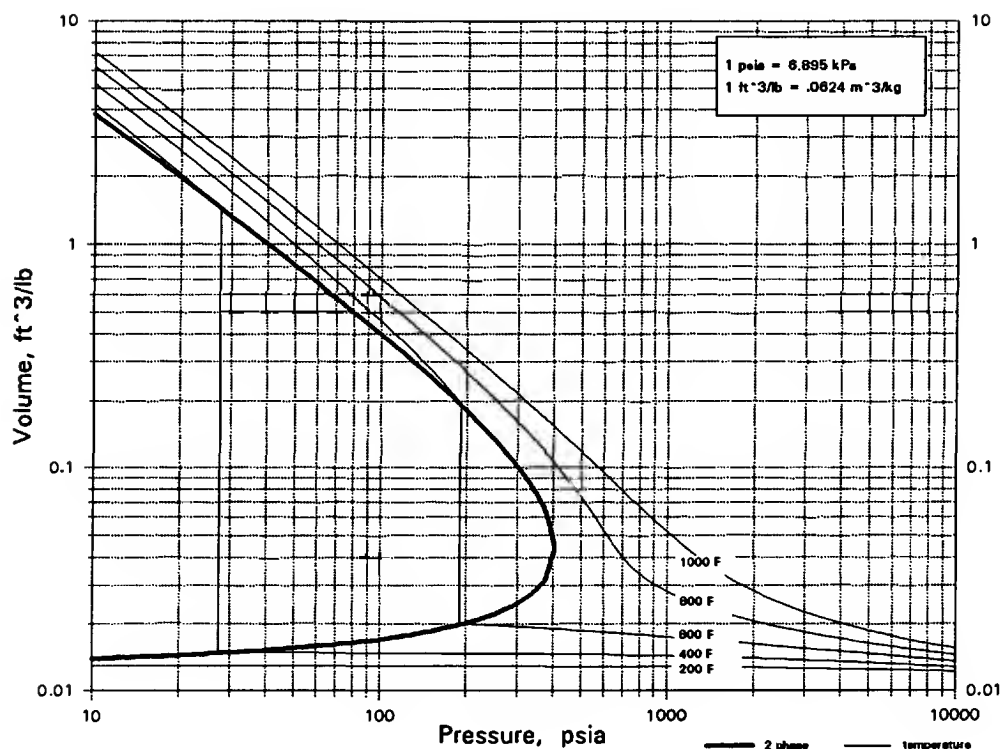
C7H3ClF3NO 24-CHLORO-3-NITROBENZOTRIFLUORIDE



Default: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

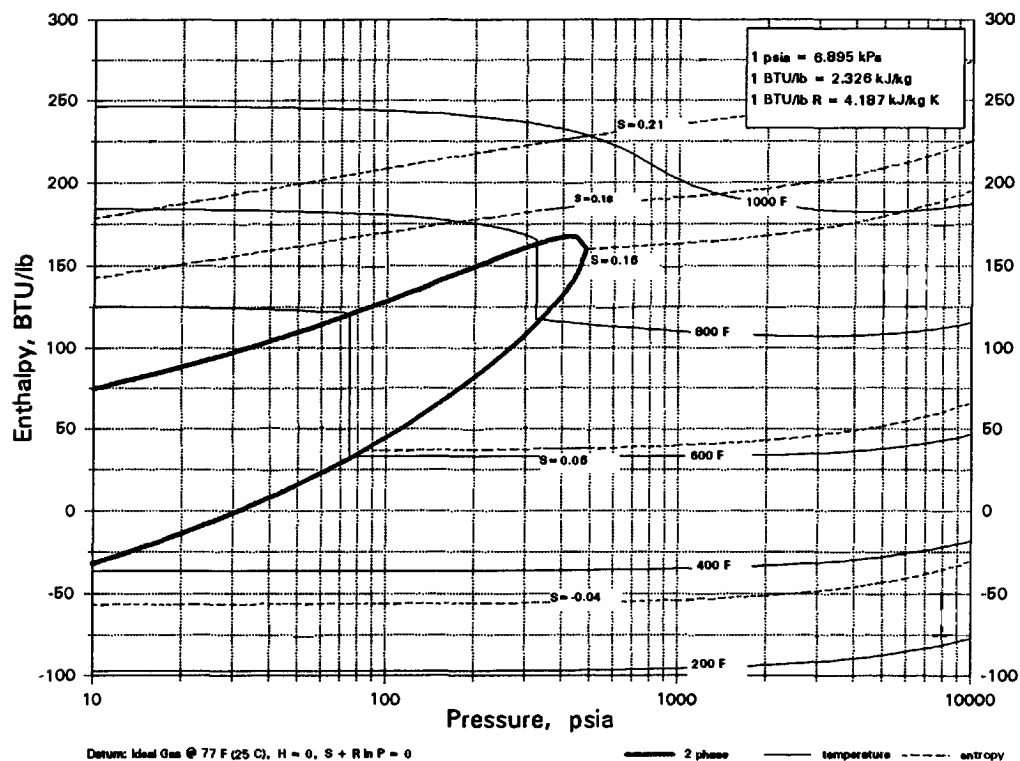
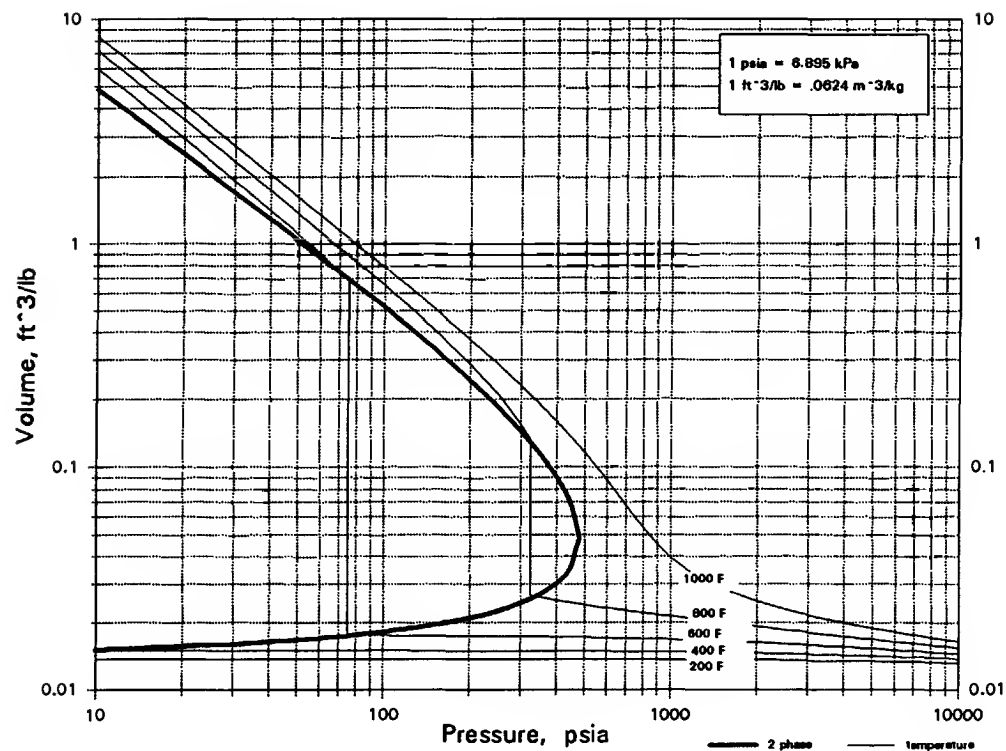
C7H3Cl2F3

2,4-DICHLOROBENZOTRIFLUORIDE



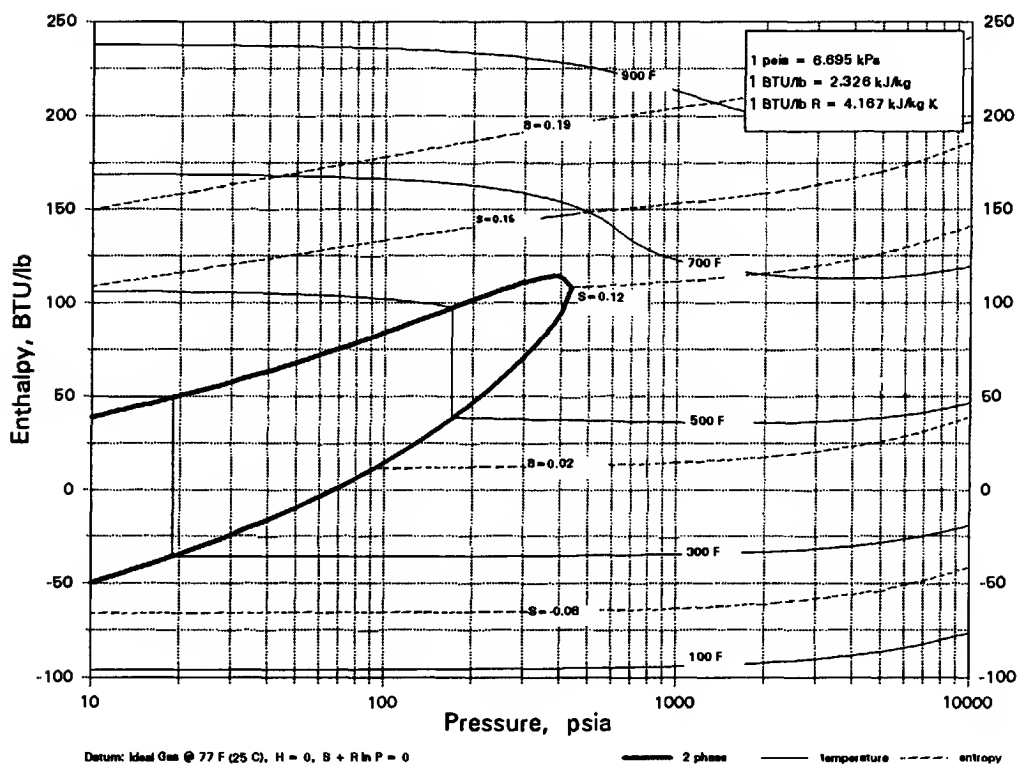
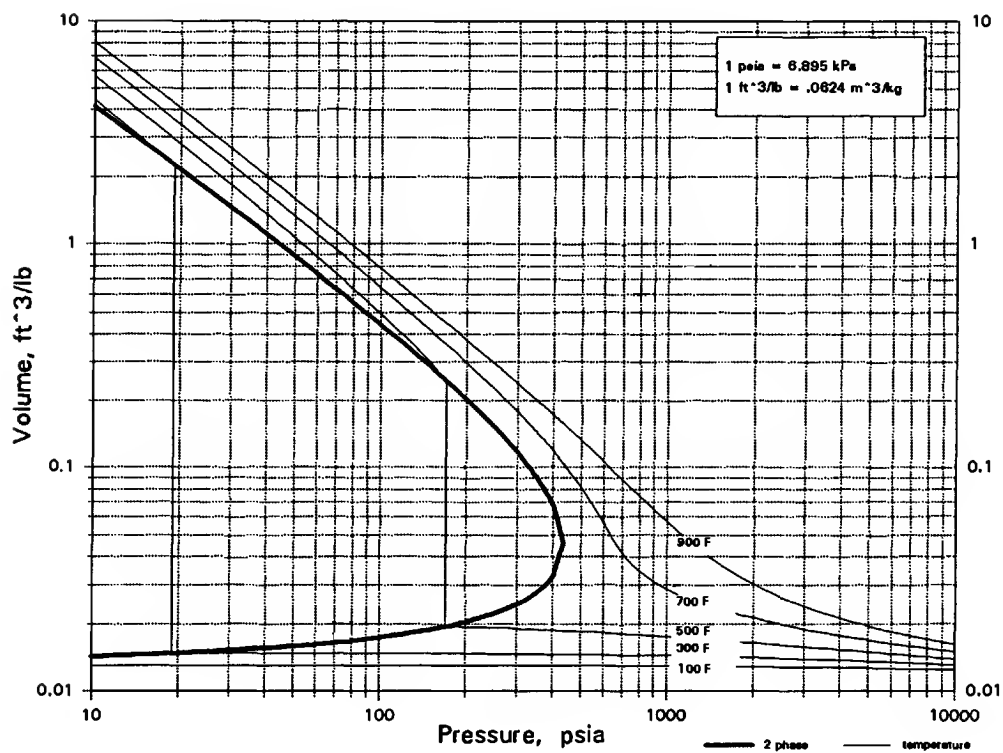
C7H3Cl2NO

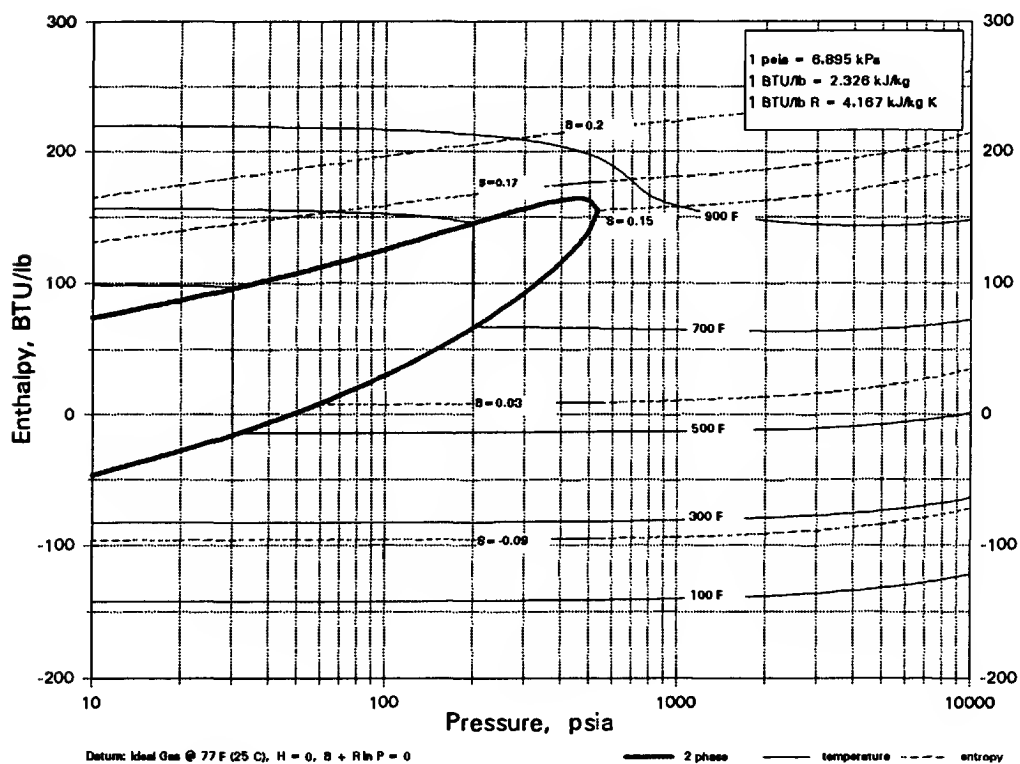
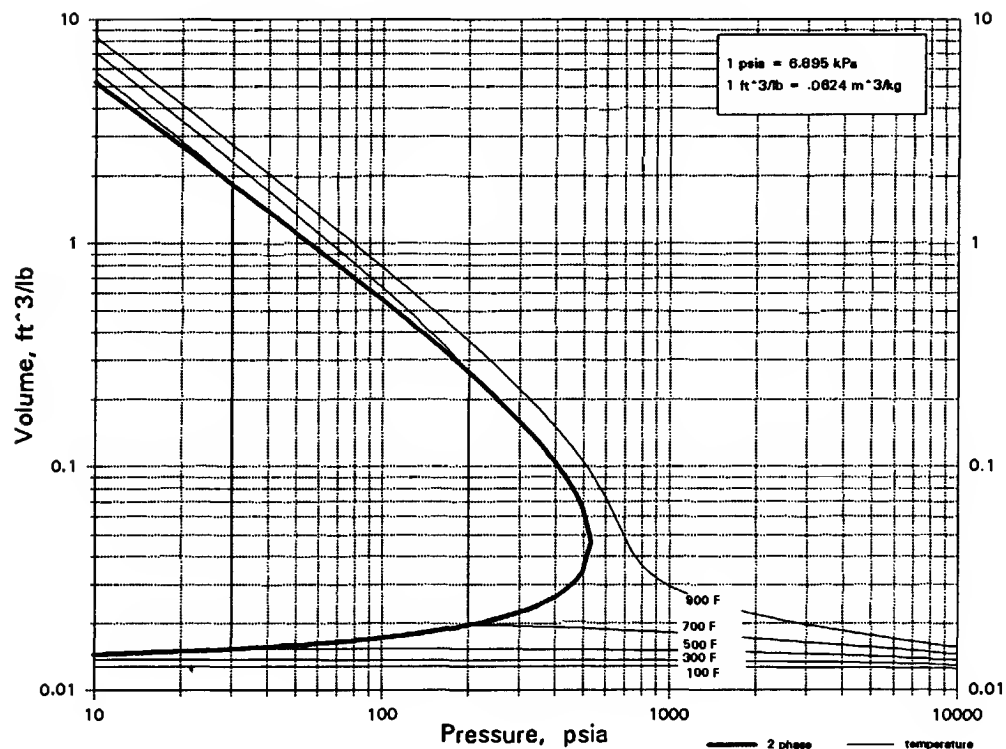
3-4-DICHLOROPHENYL ISOCYANATE



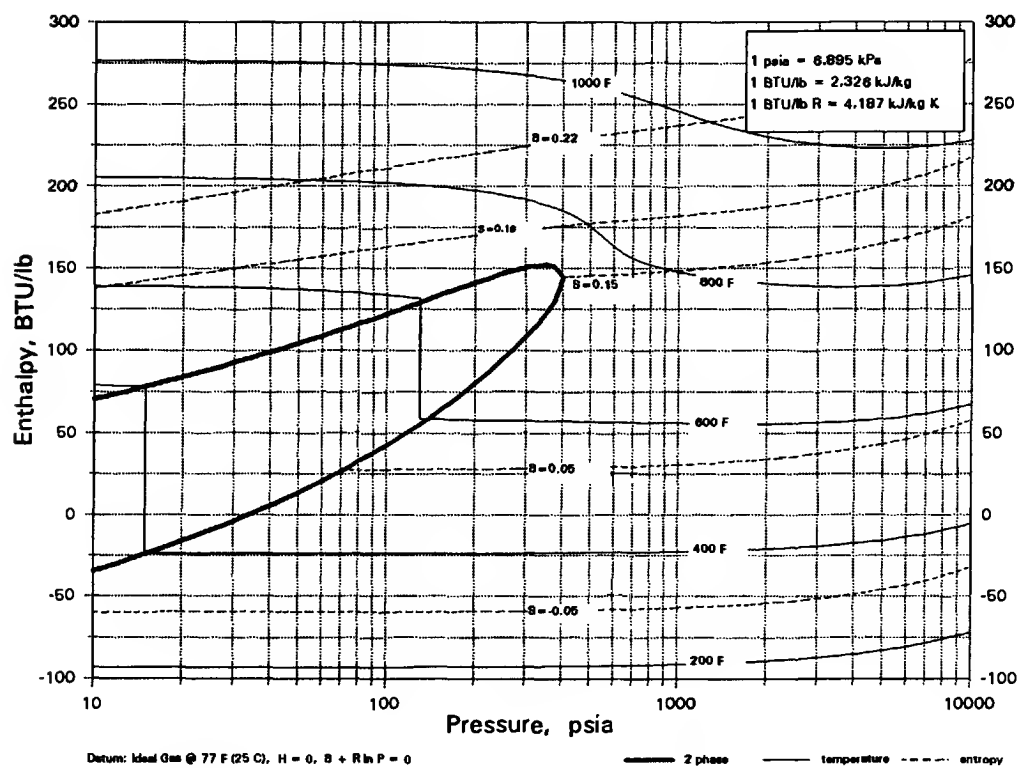
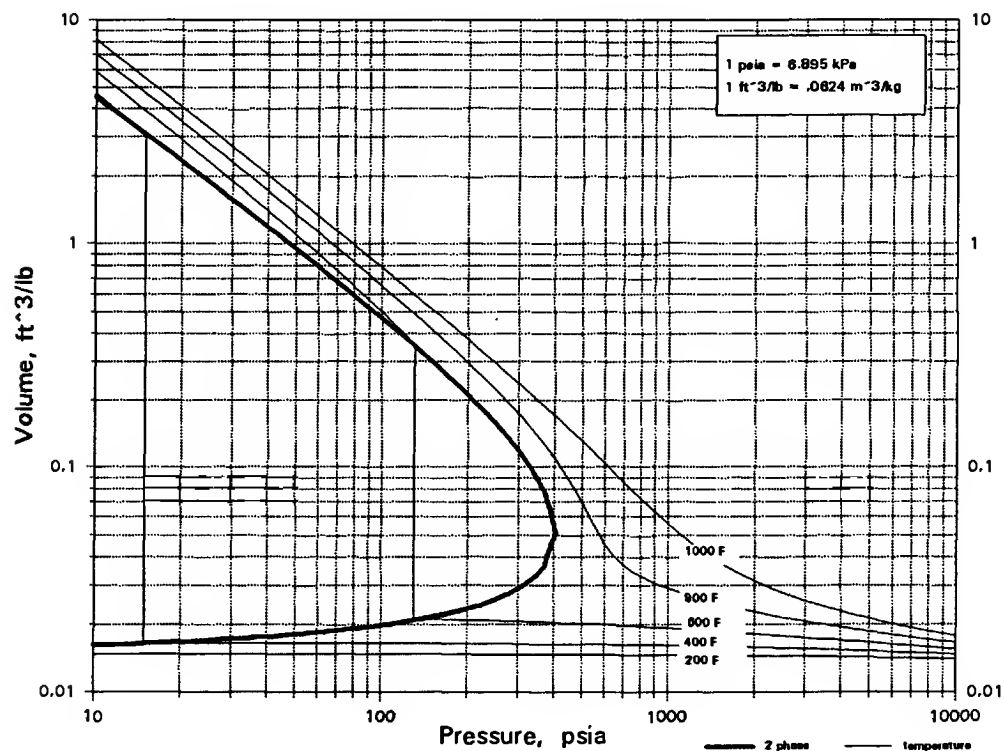
C7H4ClF3

p-CHLORO BENZOTRIFLUORIDE



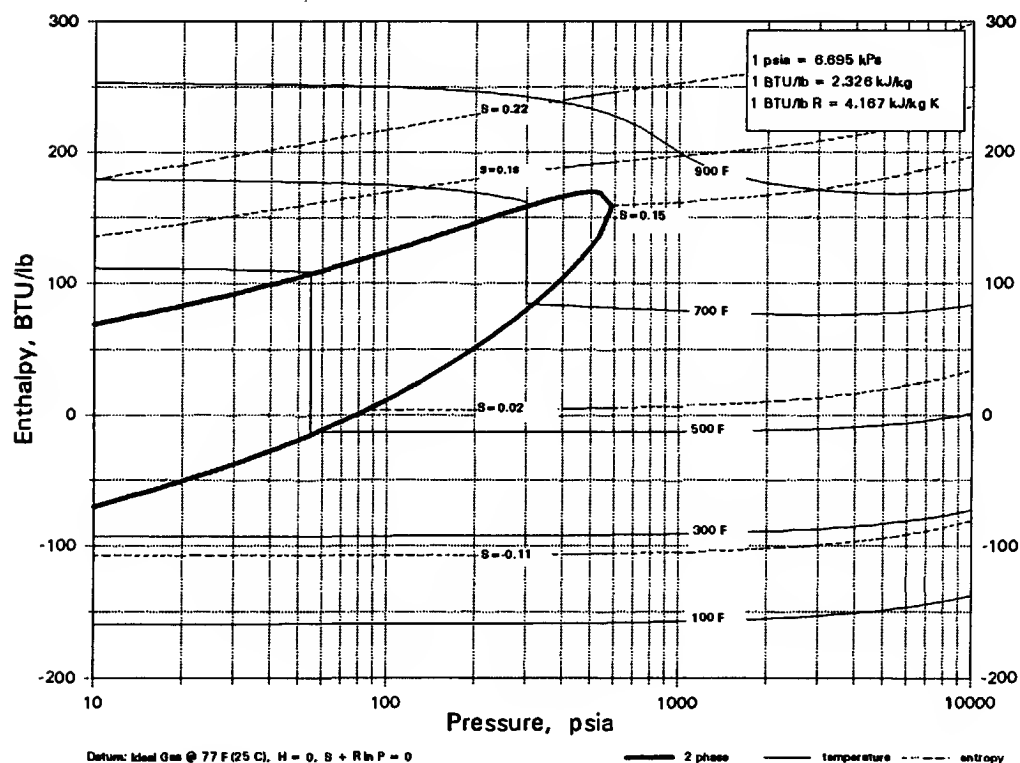
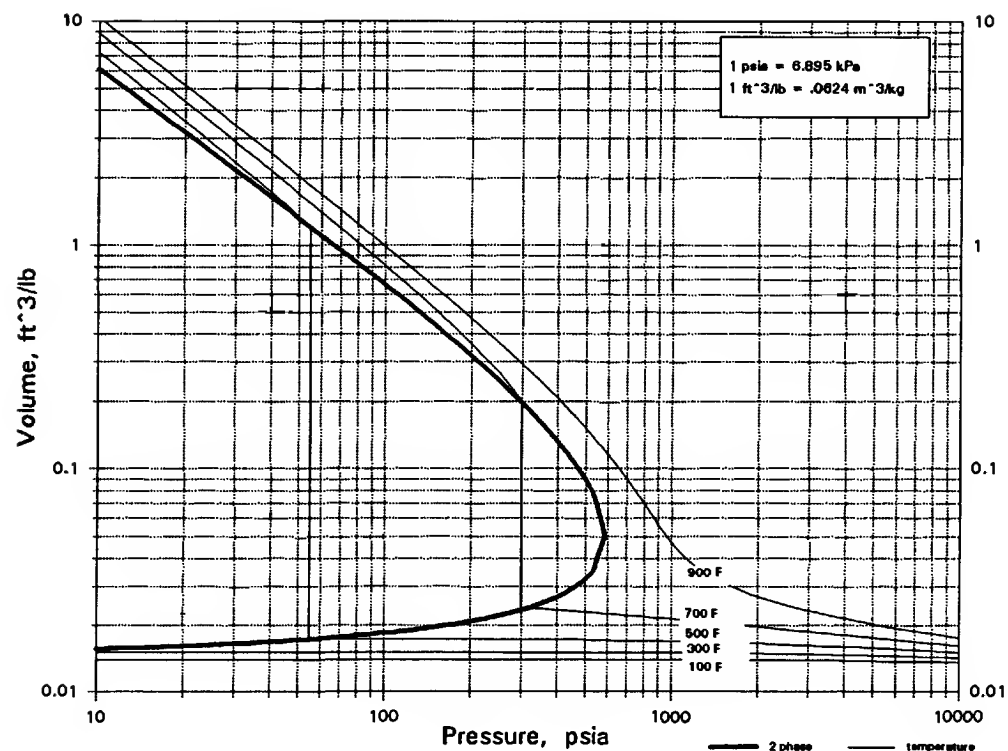
C7H4Cl2O**m-CHLOROBENZOYL CHLORIDE**

C7H4F3NO2 3-NITROBENZOTRIFLUORIDE

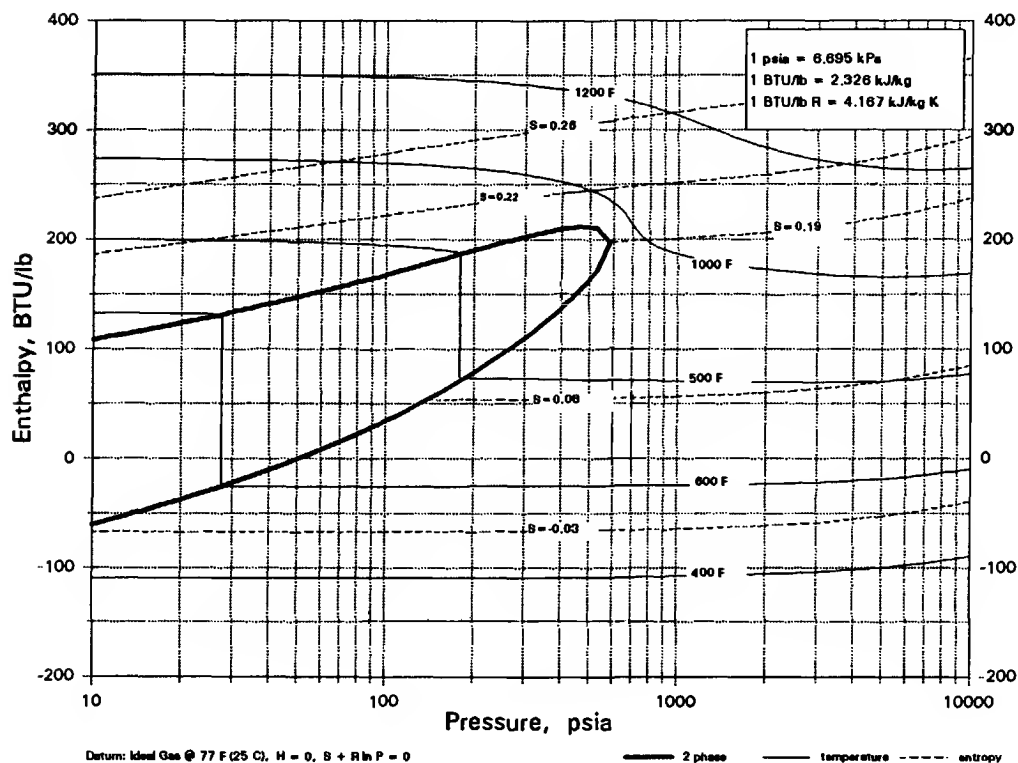
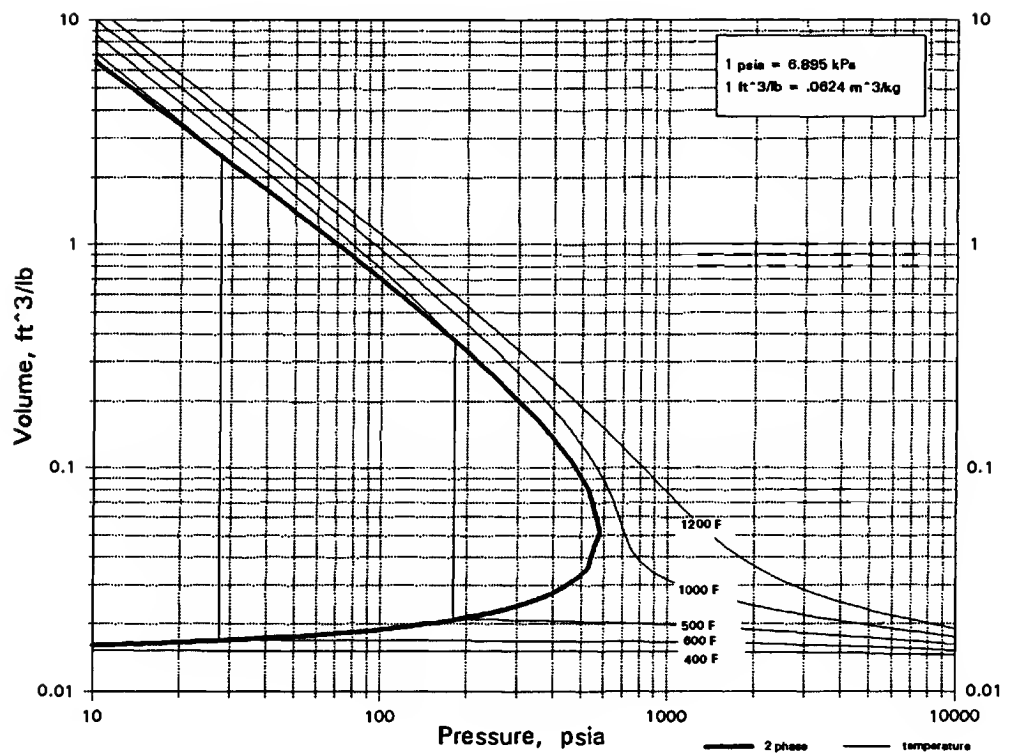


C7H5ClO

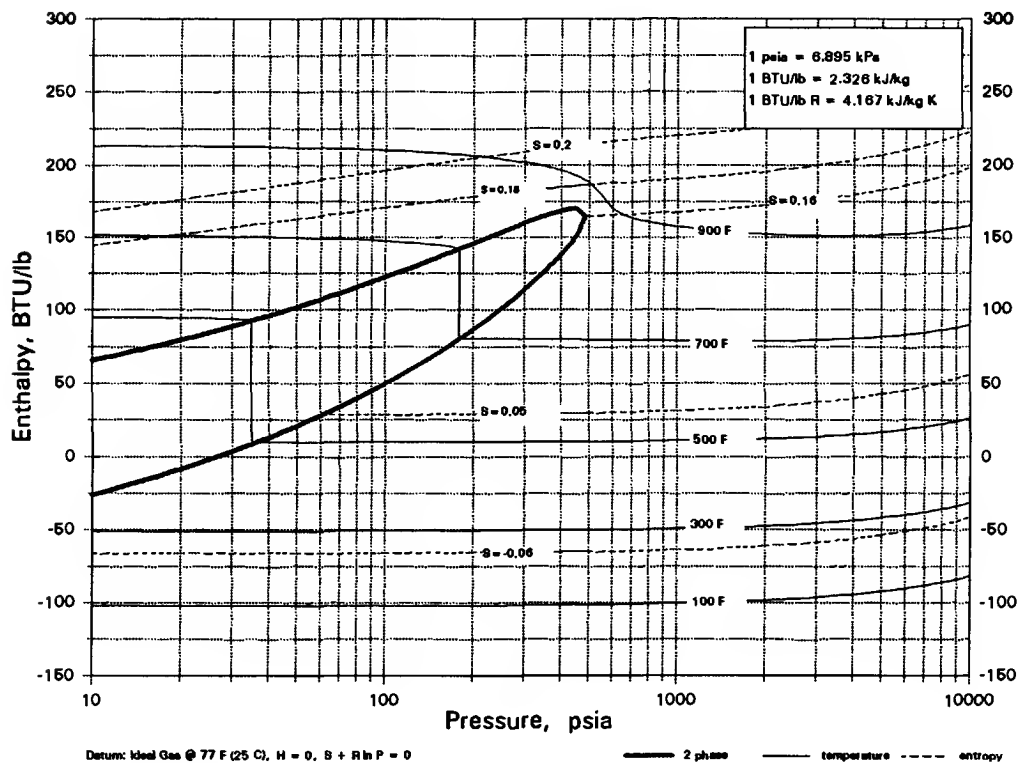
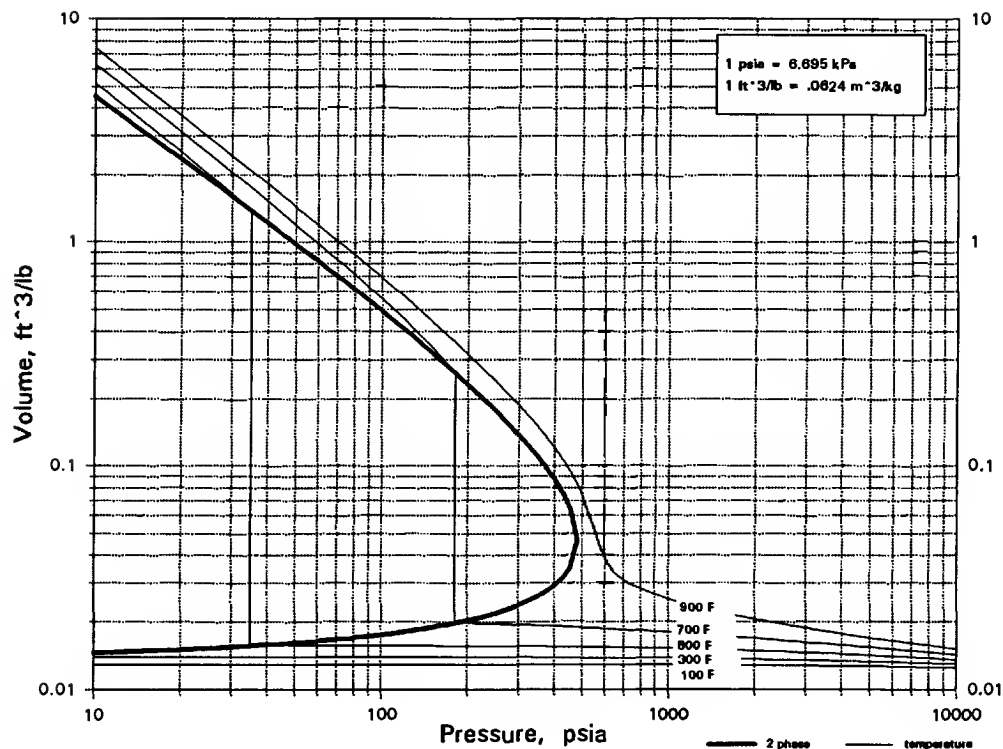
BENZOYL CHLORIDE



$C_7H_5ClO_2$ o-CHLOROBENZOIC ACID

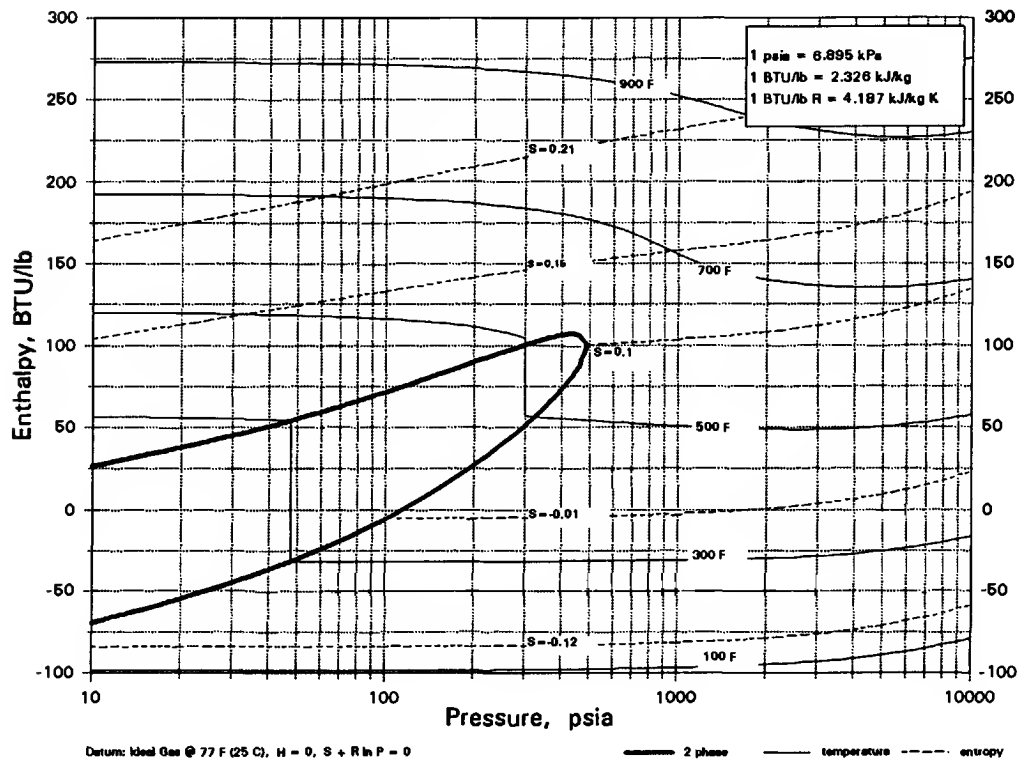
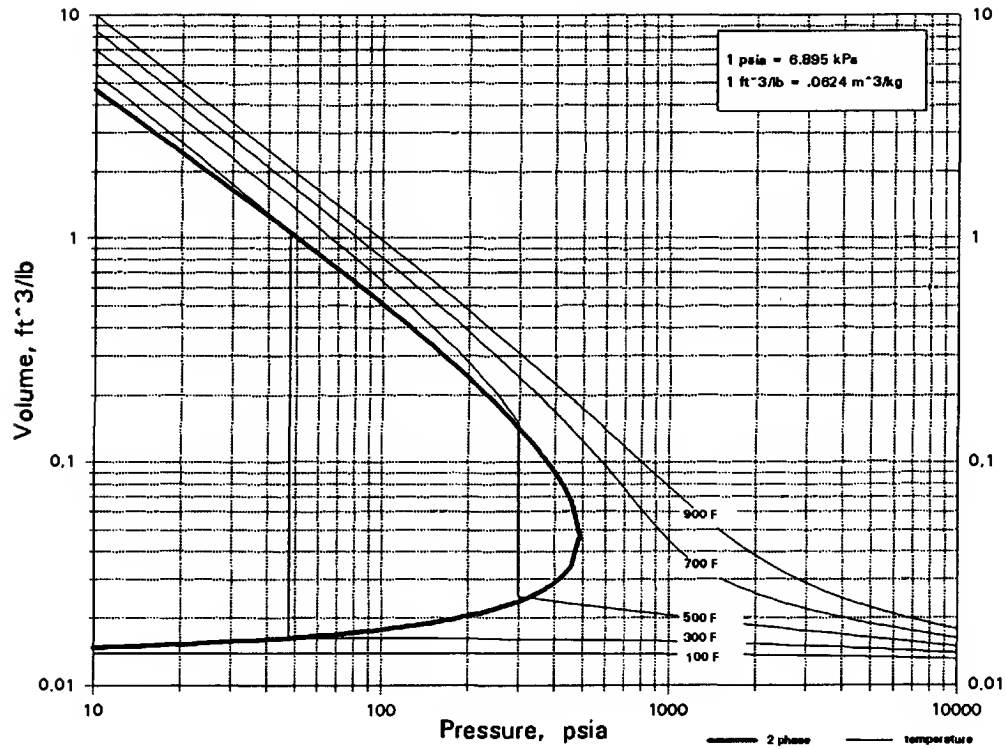


C7H5Cl3
BENZOTRICHLORIDE



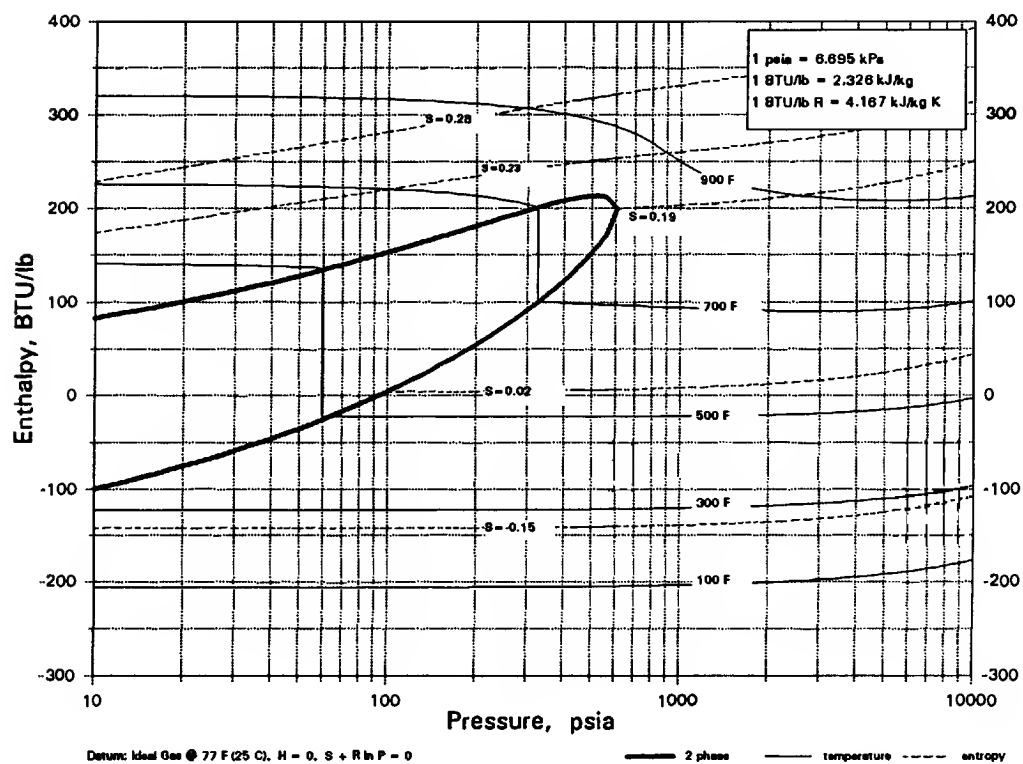
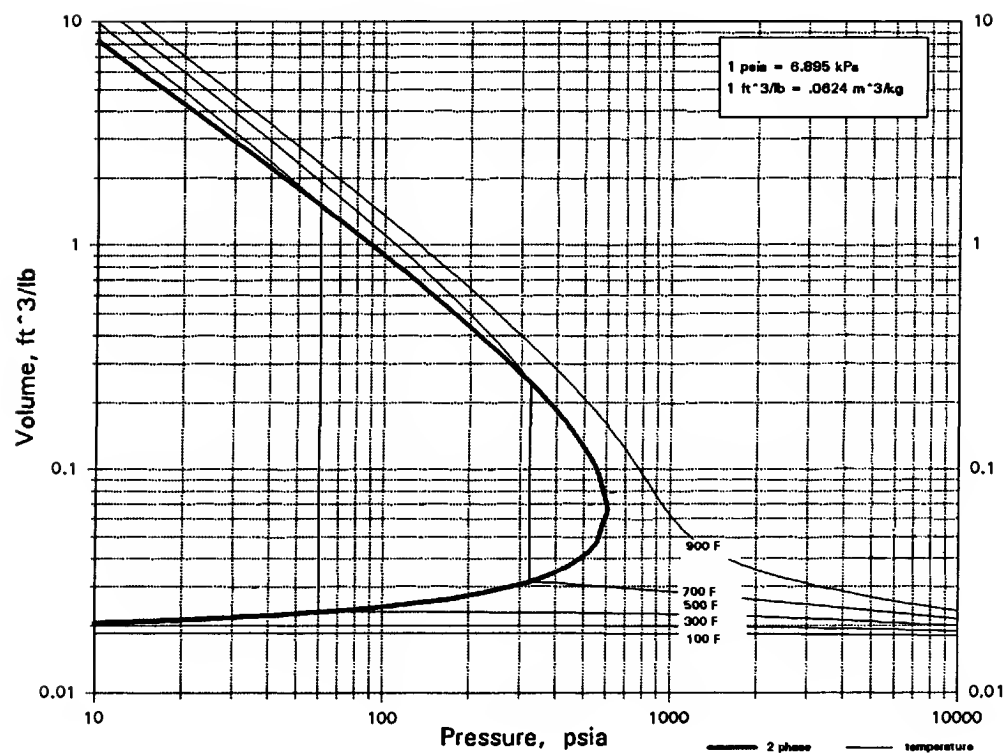
C7H5F3

BENZOTRIFLUORIDE



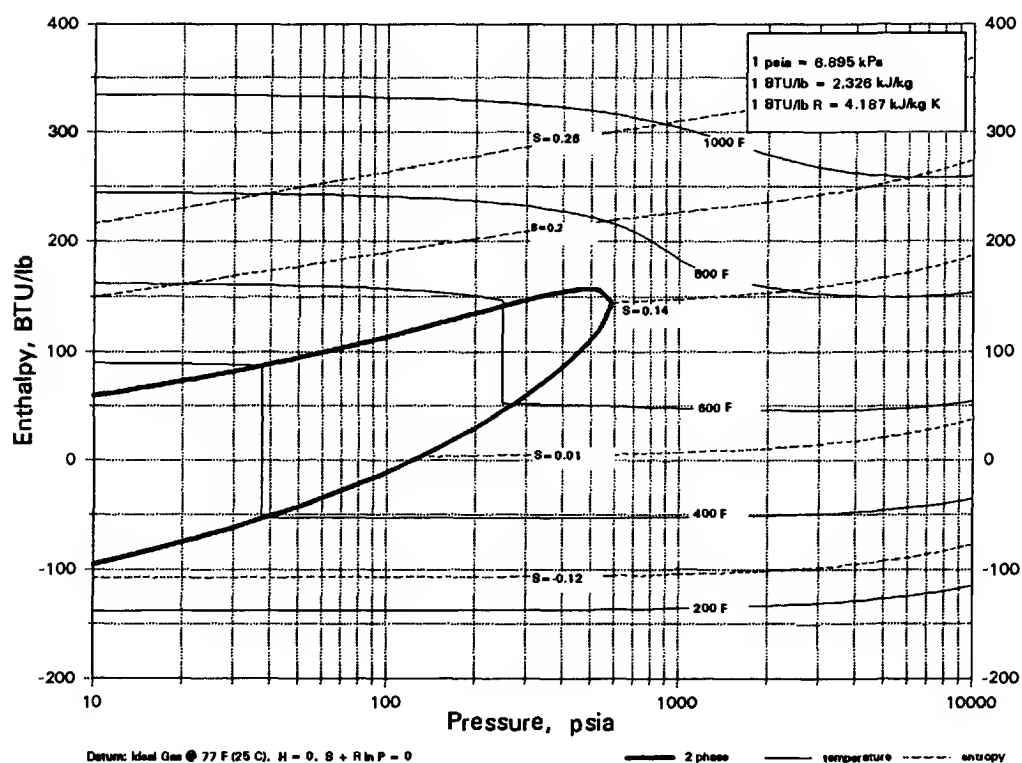
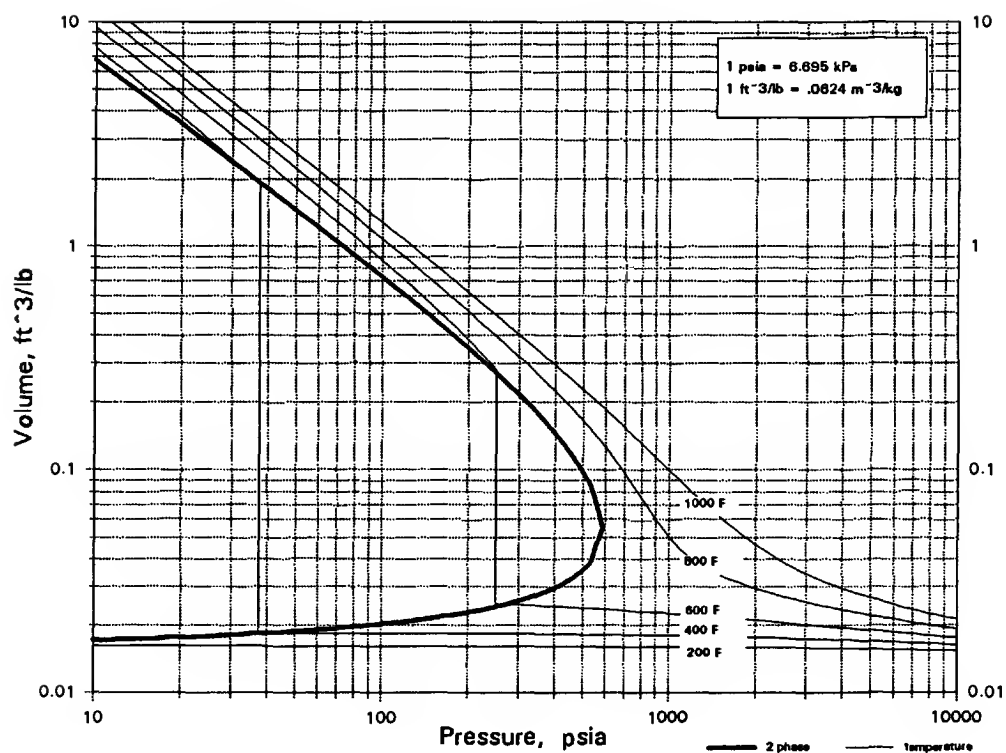
C7H5N

BENZONITRILE

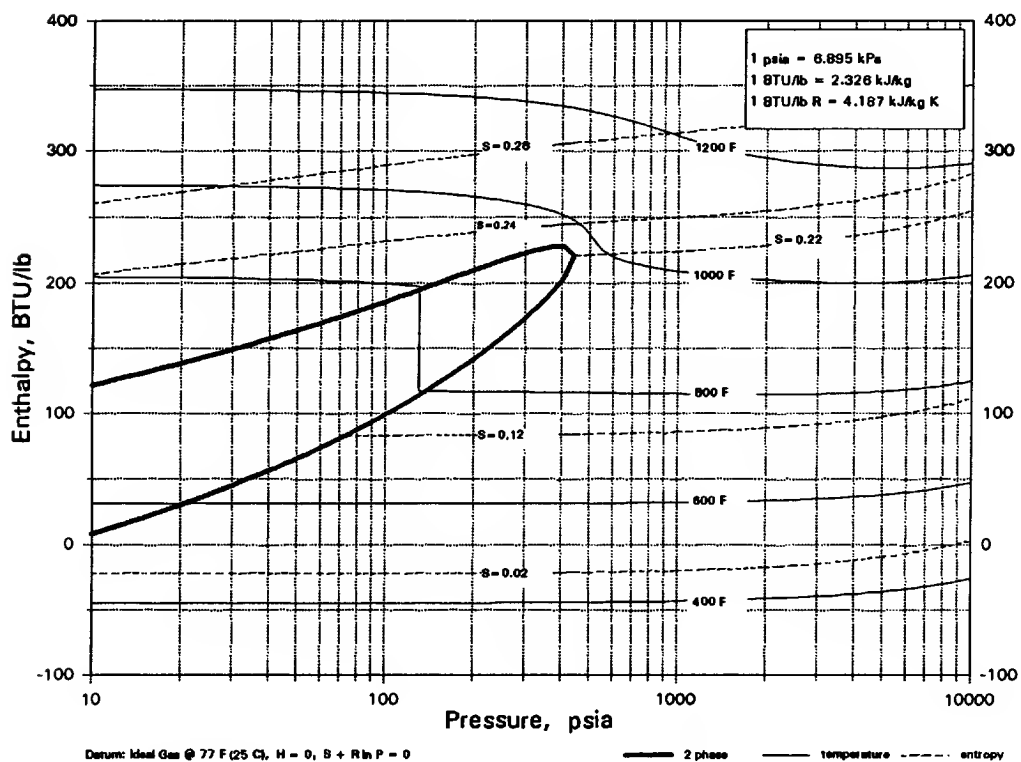
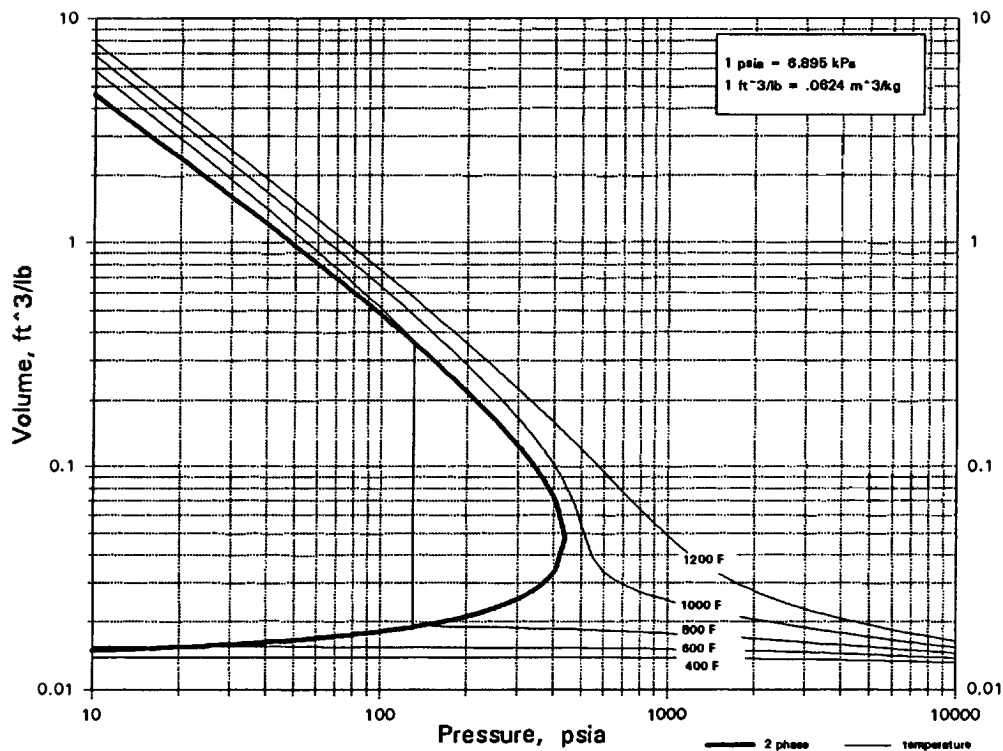


C7H5NO

PHENYL ISOCYANATE

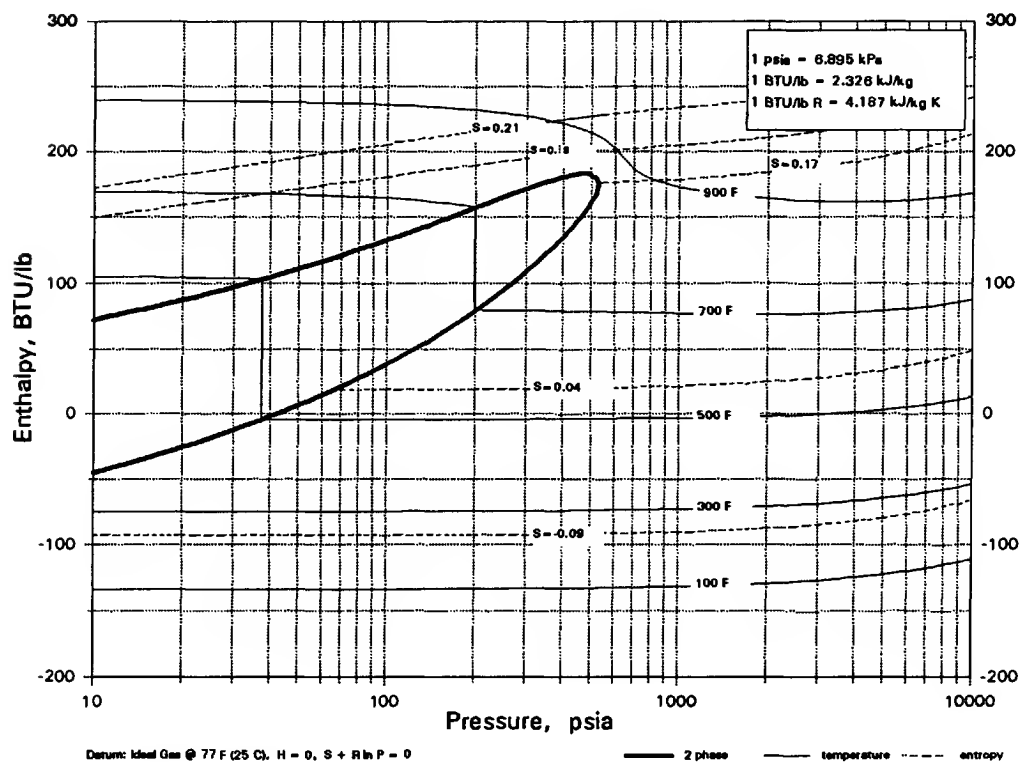
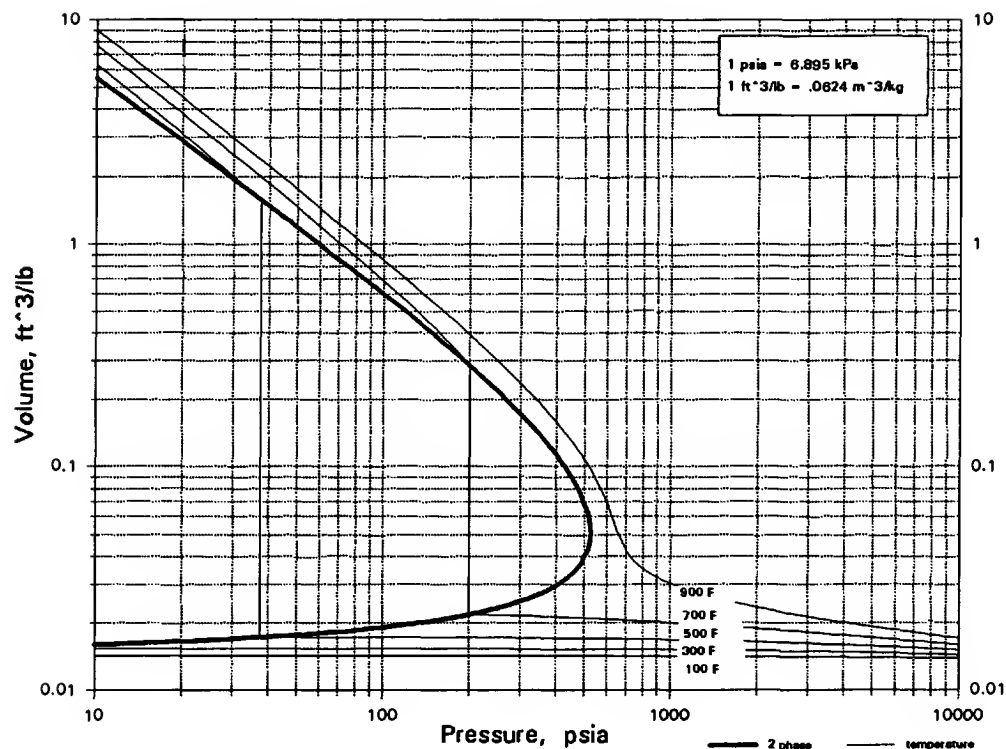


$C_7H_5N_3O_6$ 2-4-6-TRINITROTOLUENE



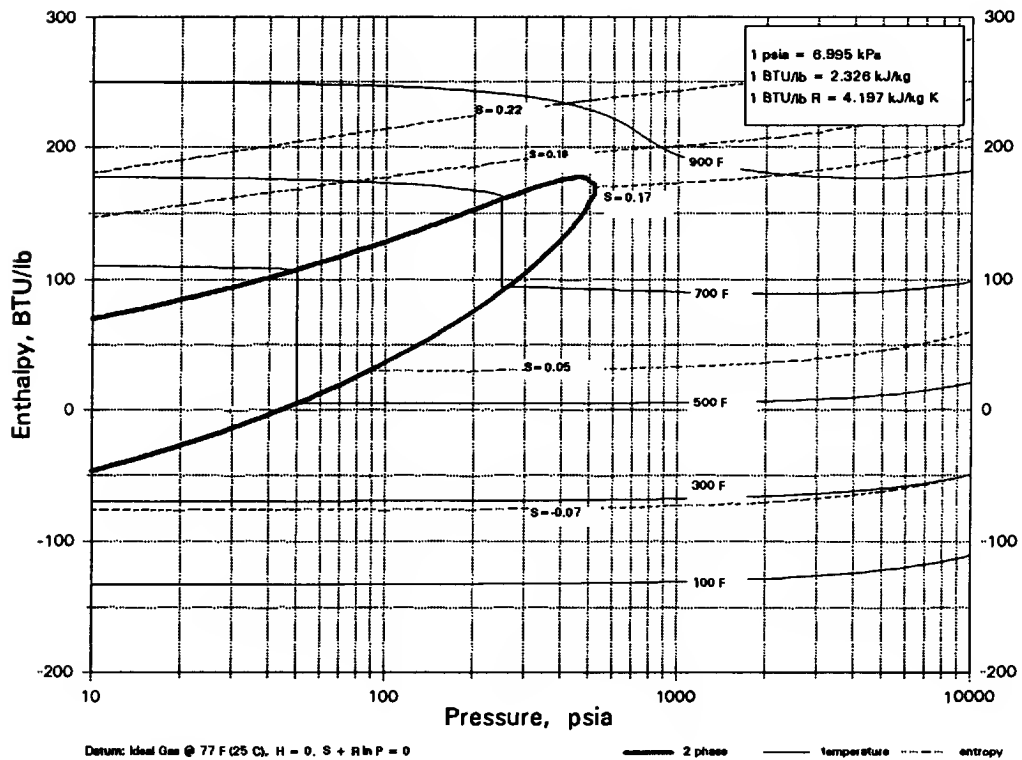
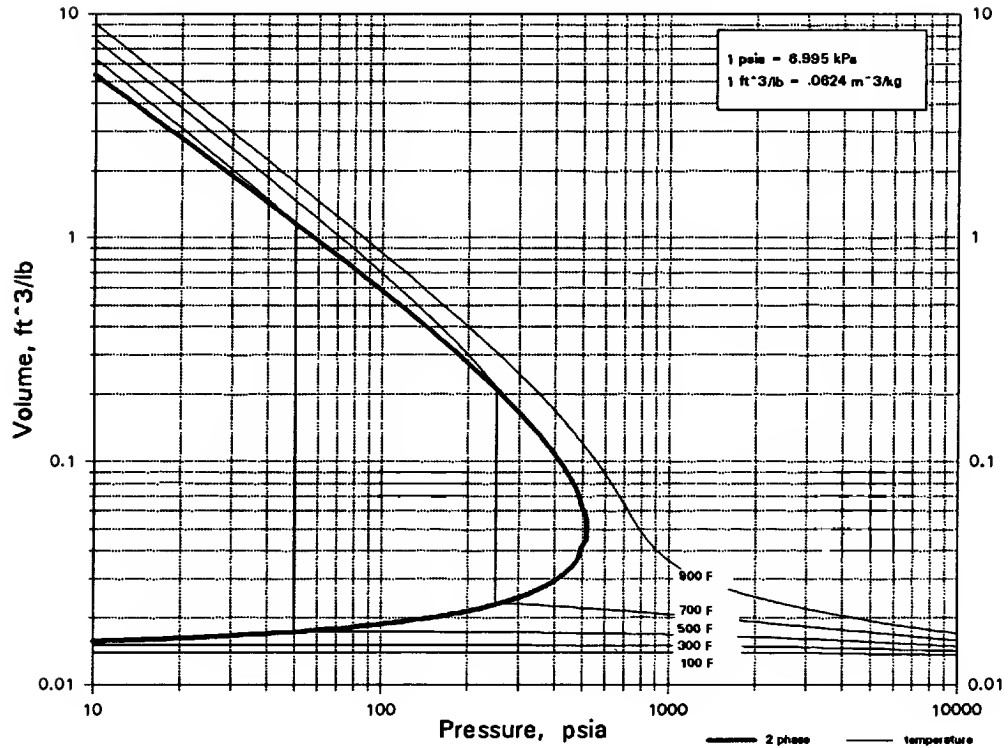
C7H6Cl2

BENZYL DICHLORIDE

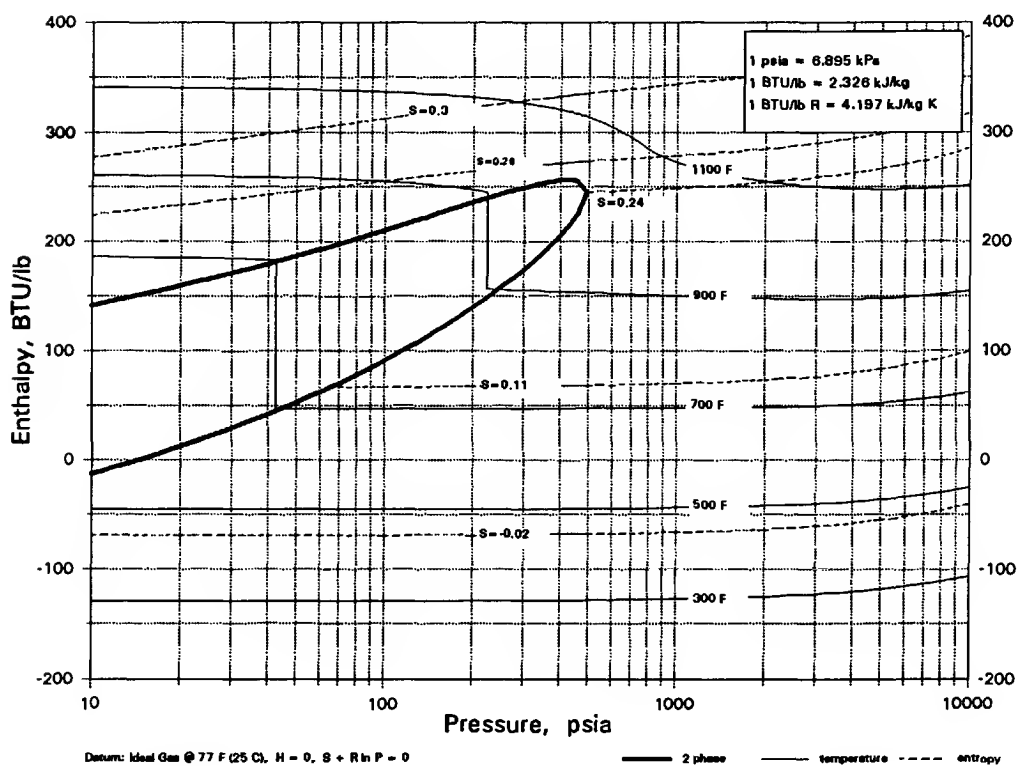
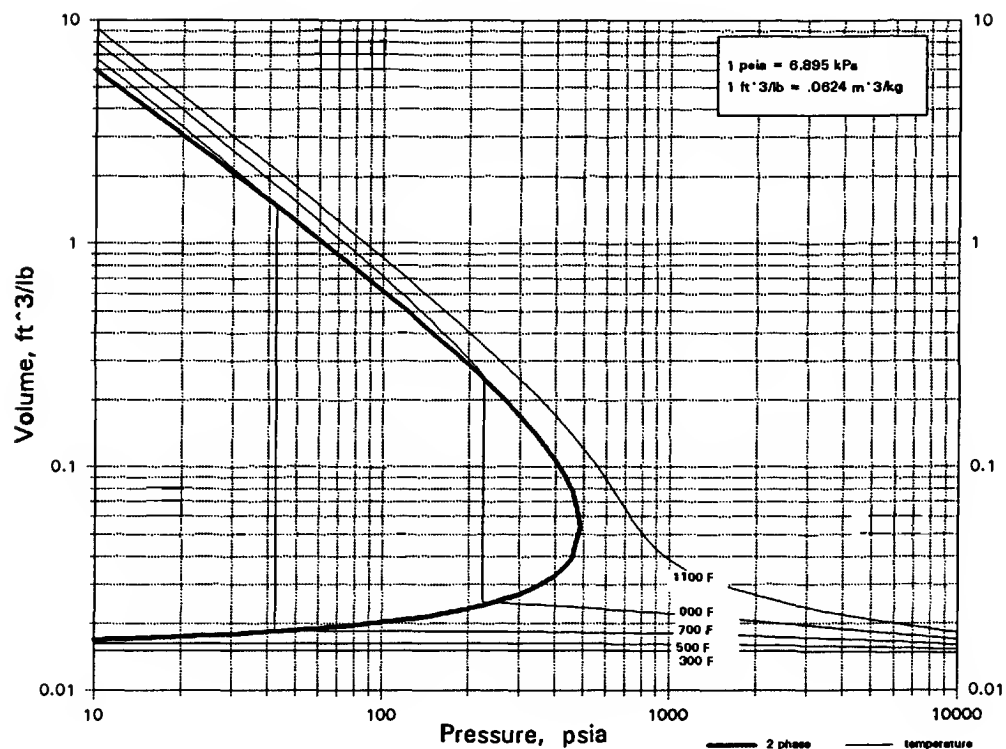


C₇H₆Cl₂

2,4-DICHLOROTOLUENE

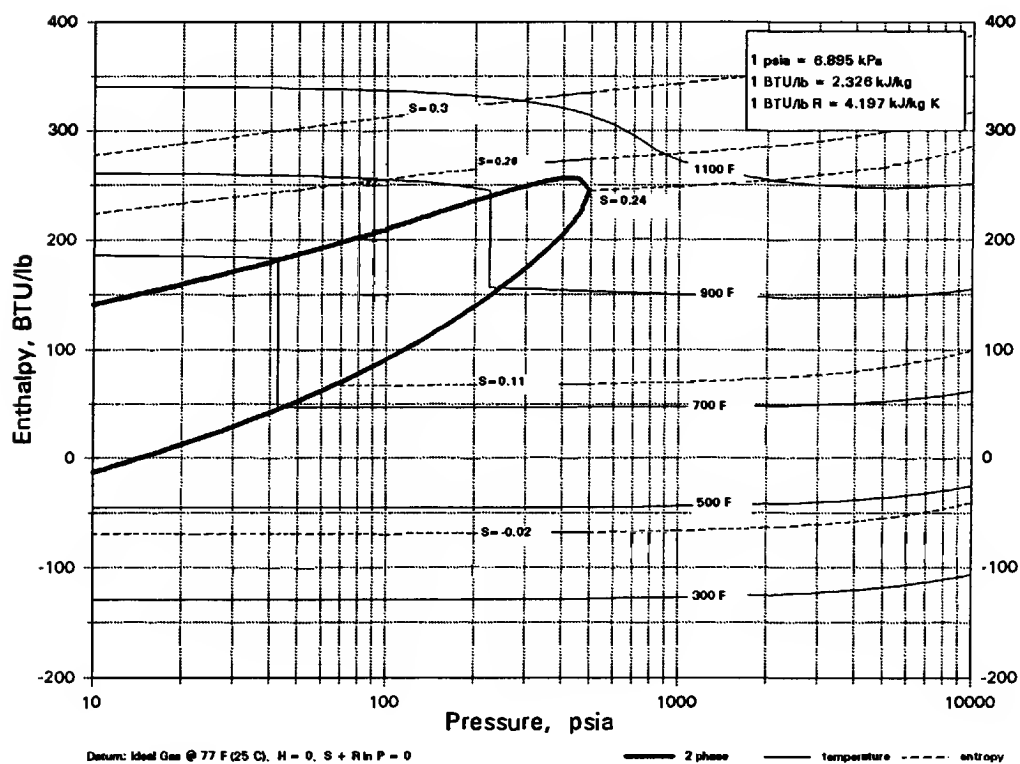
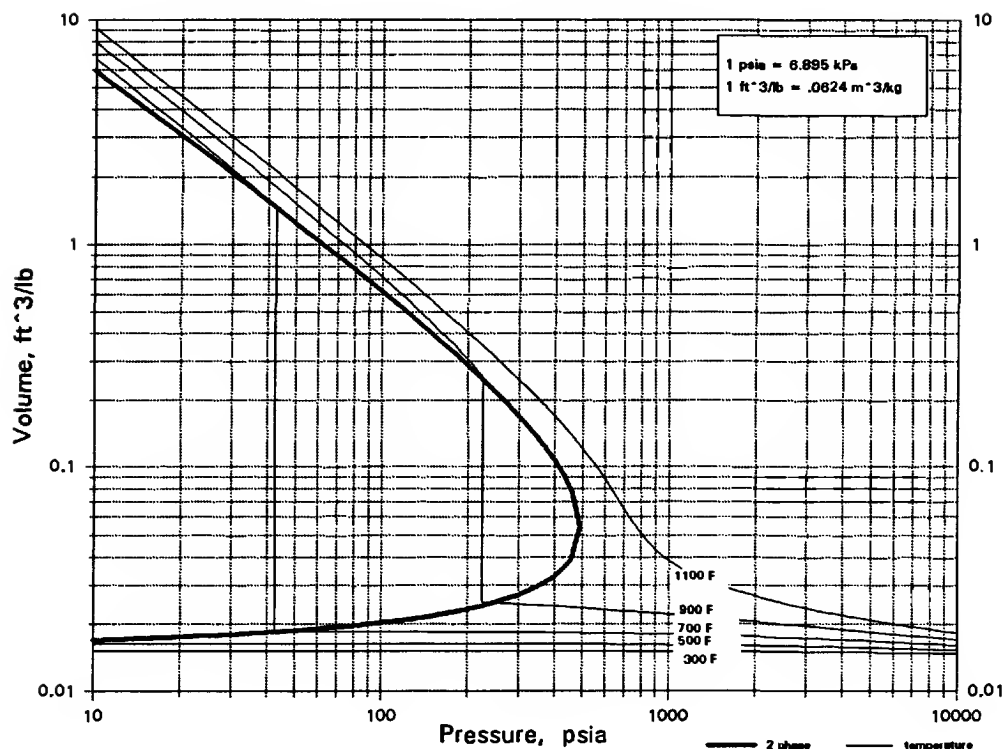


C7H6N2O4 2,4-DINITROTOLUENE



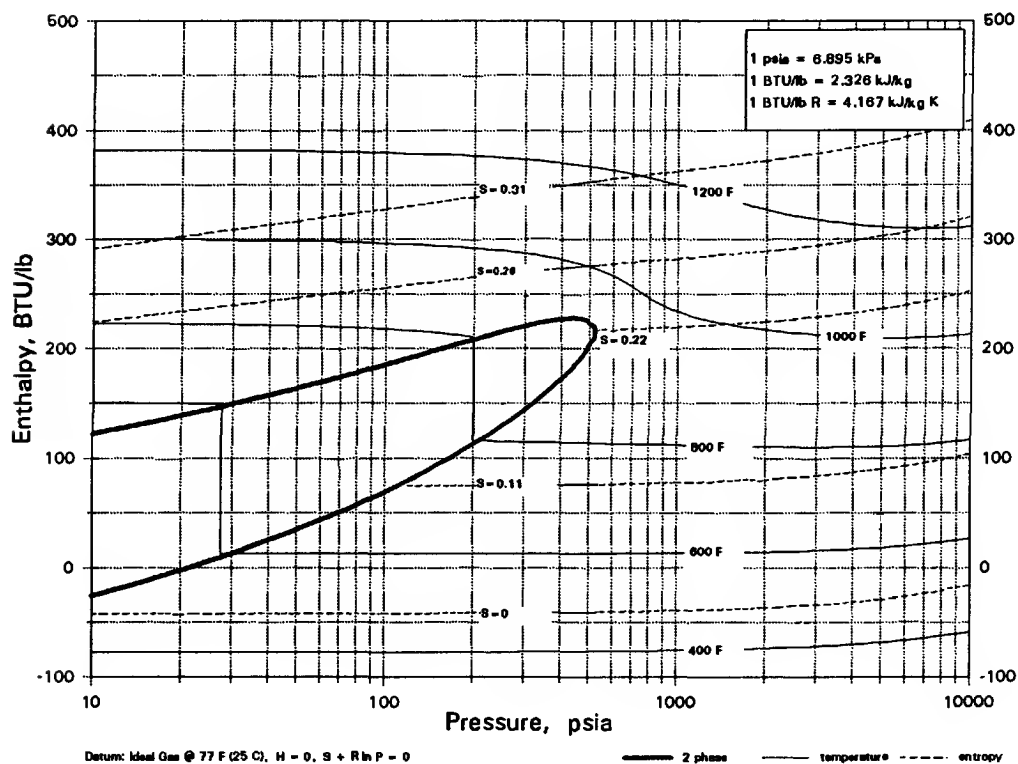
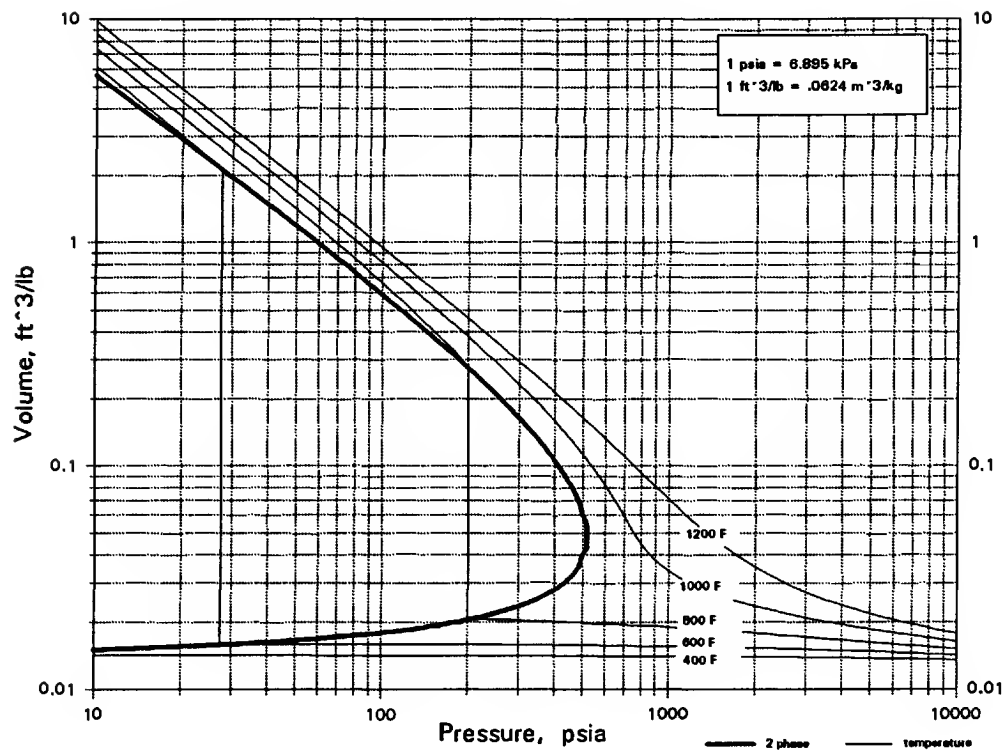
C7H6N2O4

2-5-DINITROTOLUENE



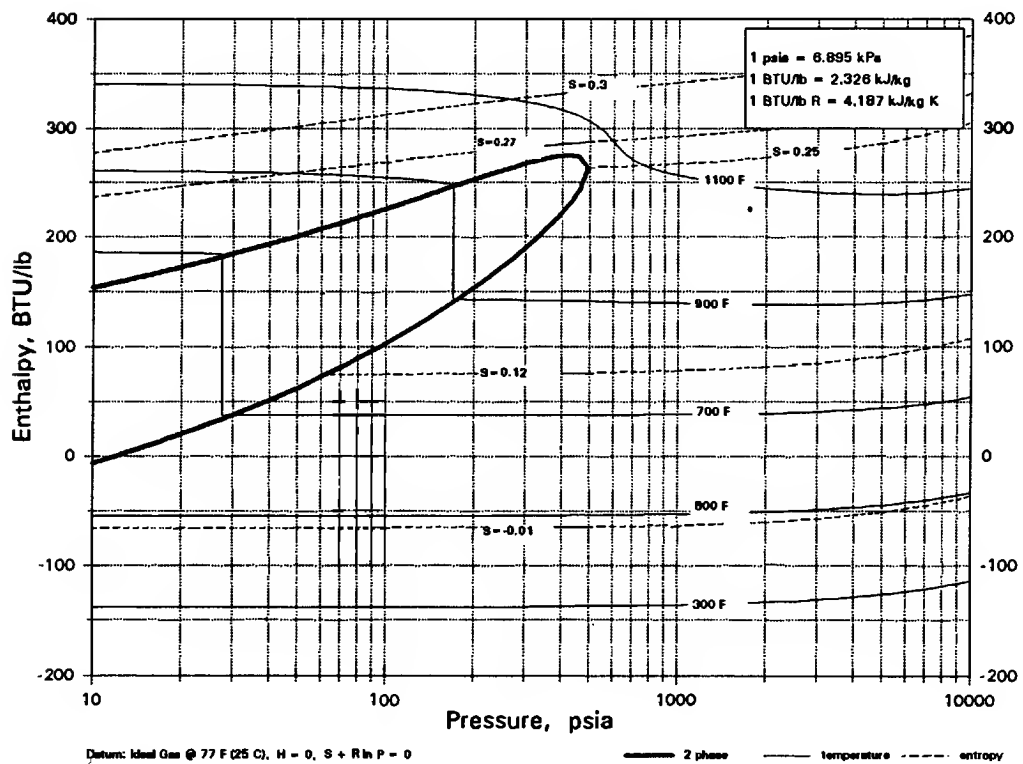
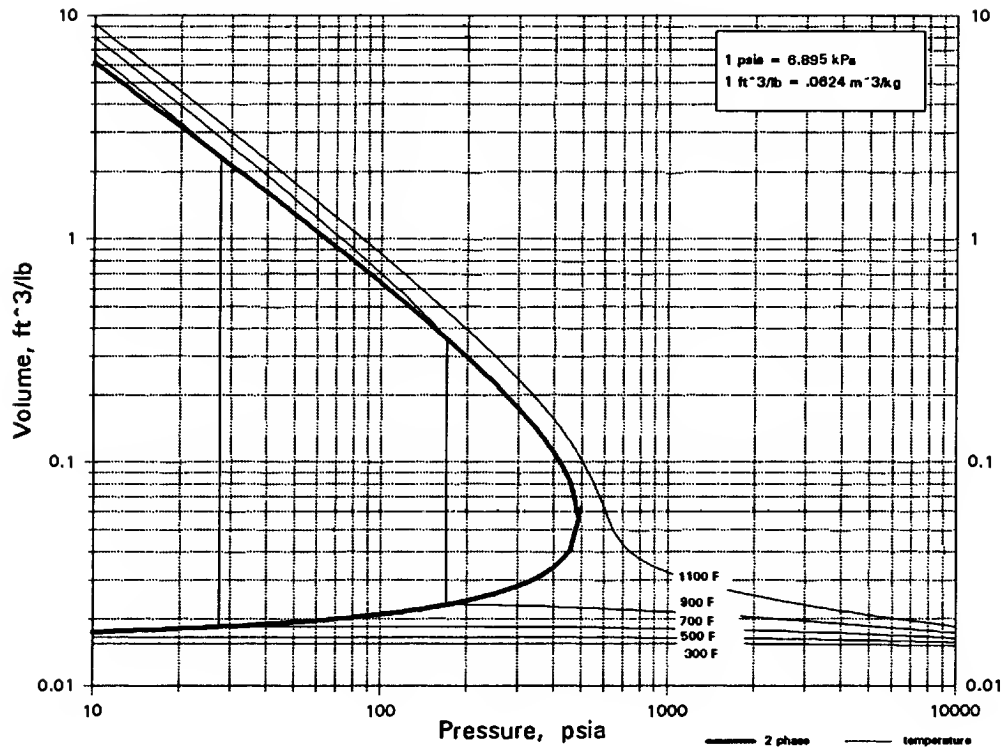
C7H6N2O4

2-6-DINITROTOLUENE



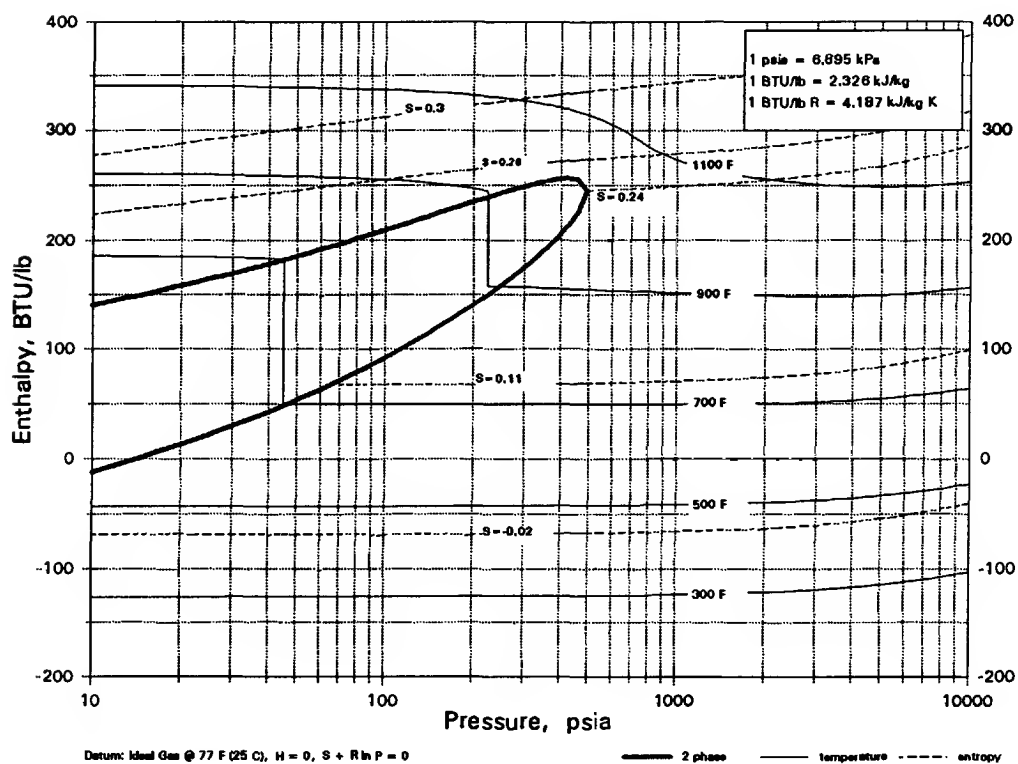
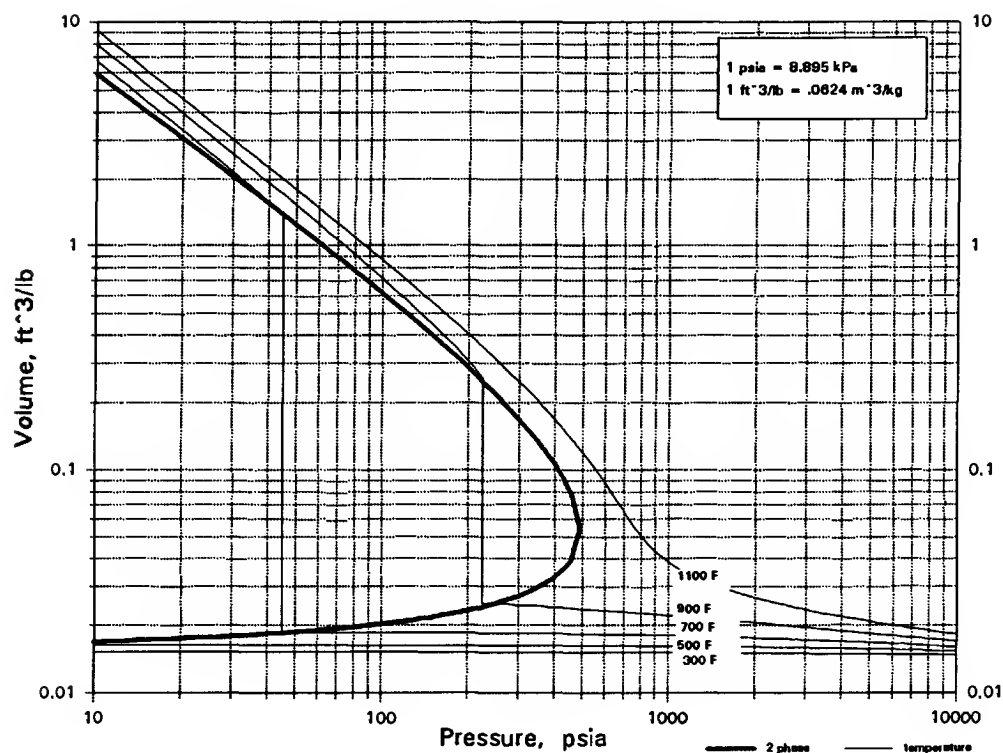
C7H6N2O4

3-4-DINITROTOLUENE



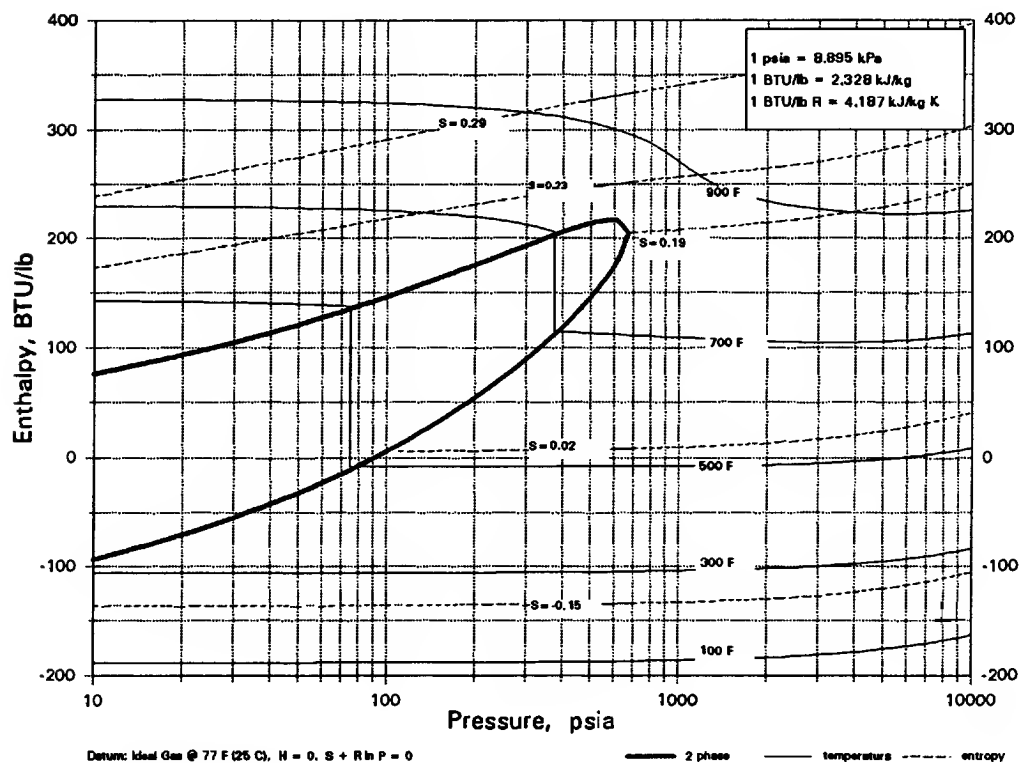
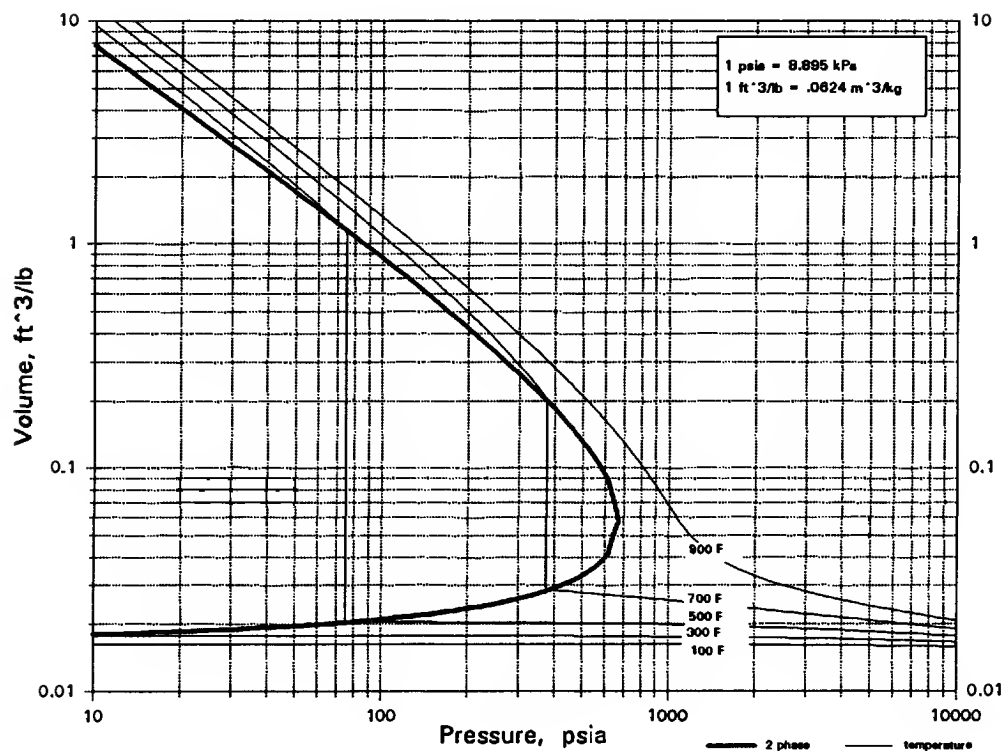
C7H6N2O4

3-5-DINITROTOLUENE



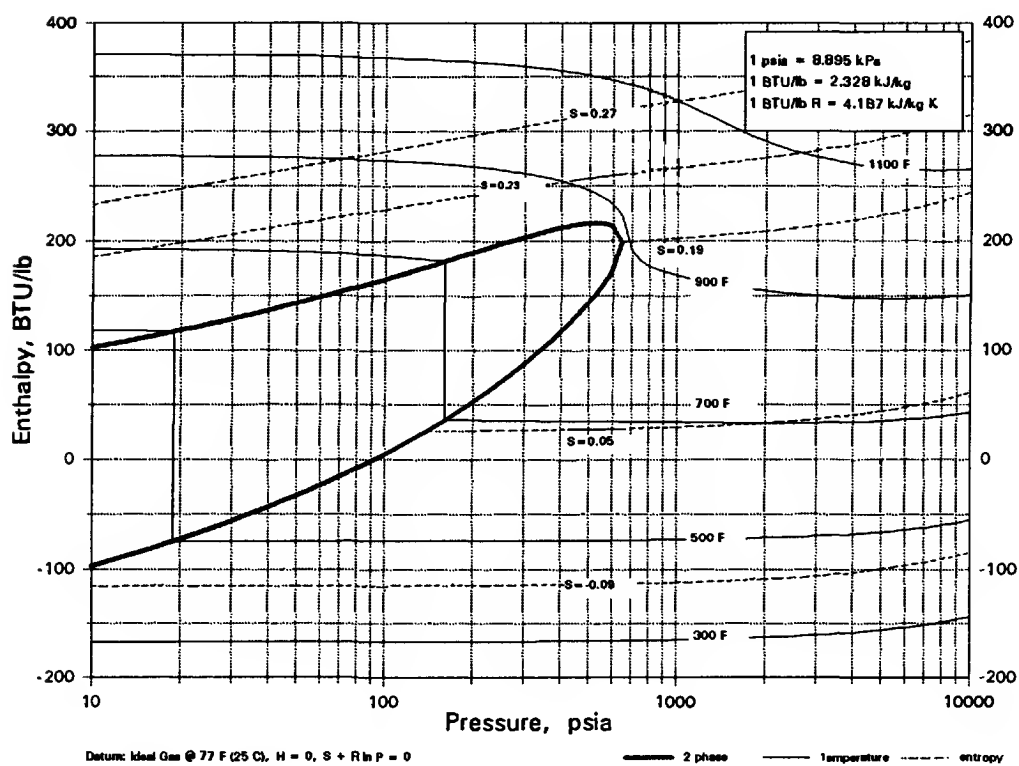
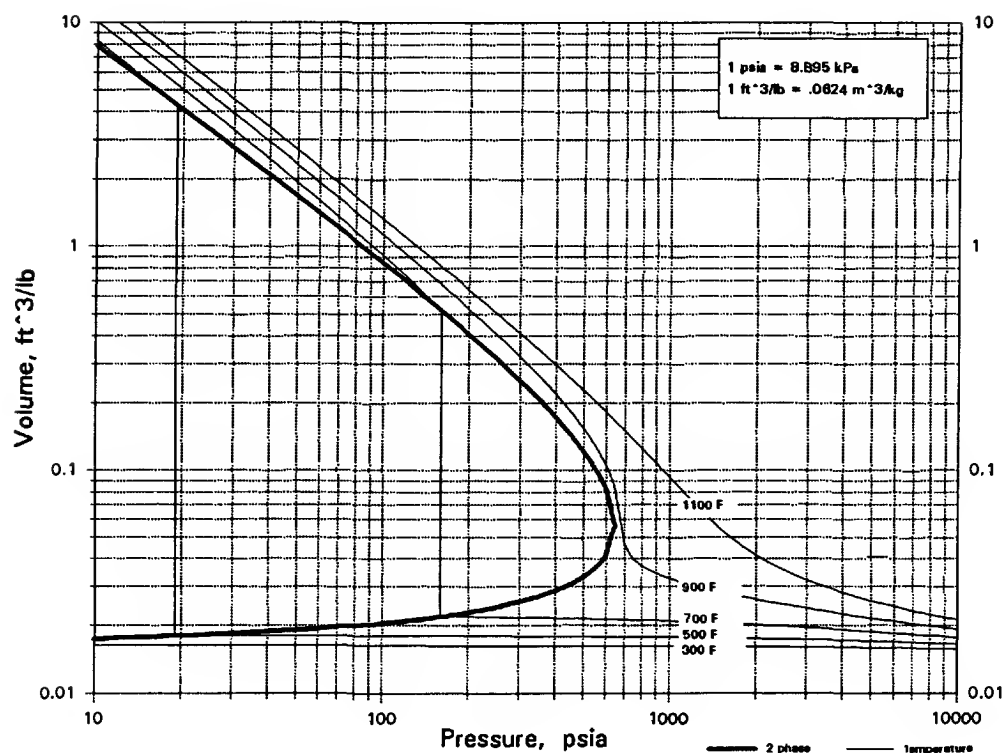
C7H6O

BENZALDEHYDE



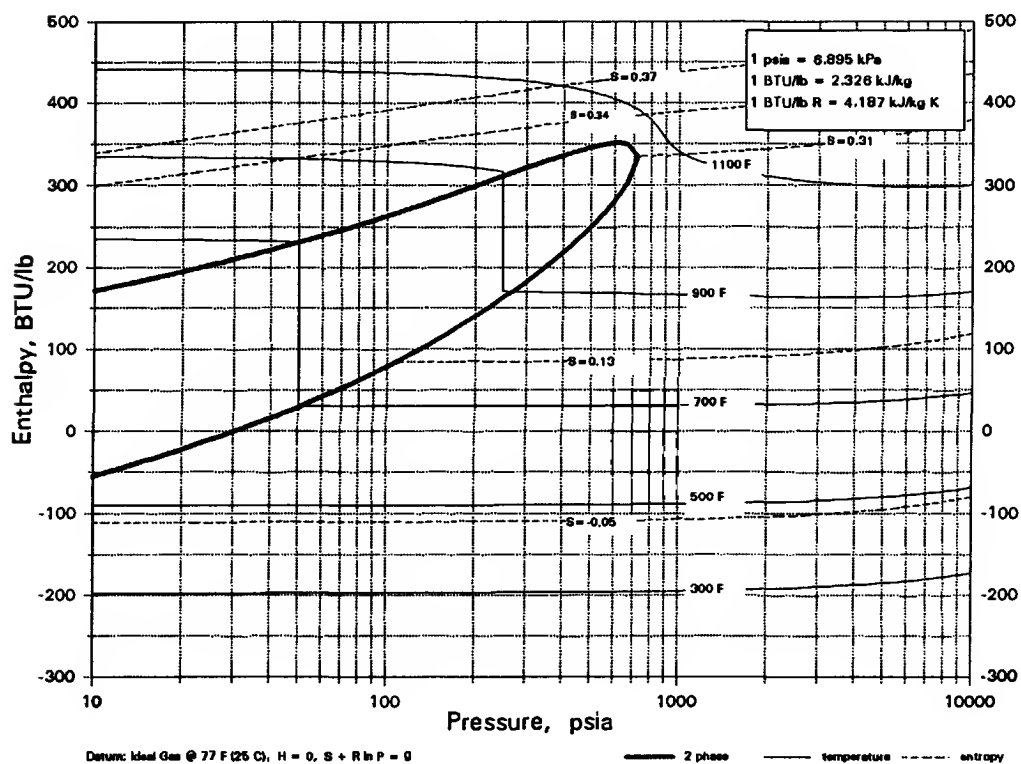
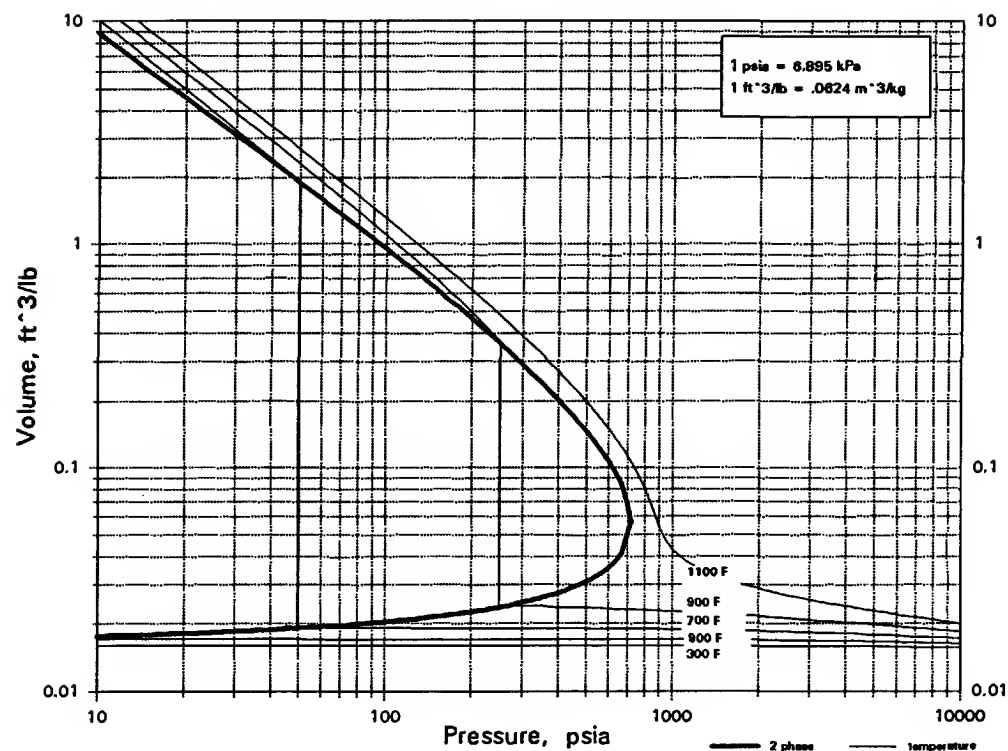
C7H6O2

BENZOIC ACID



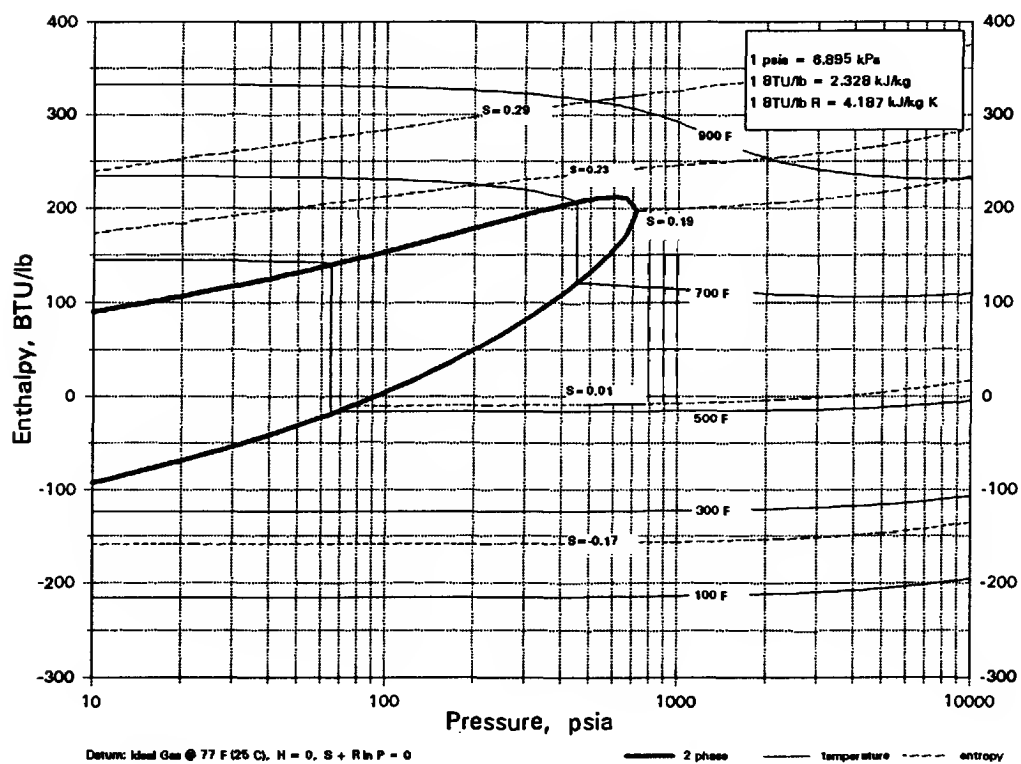
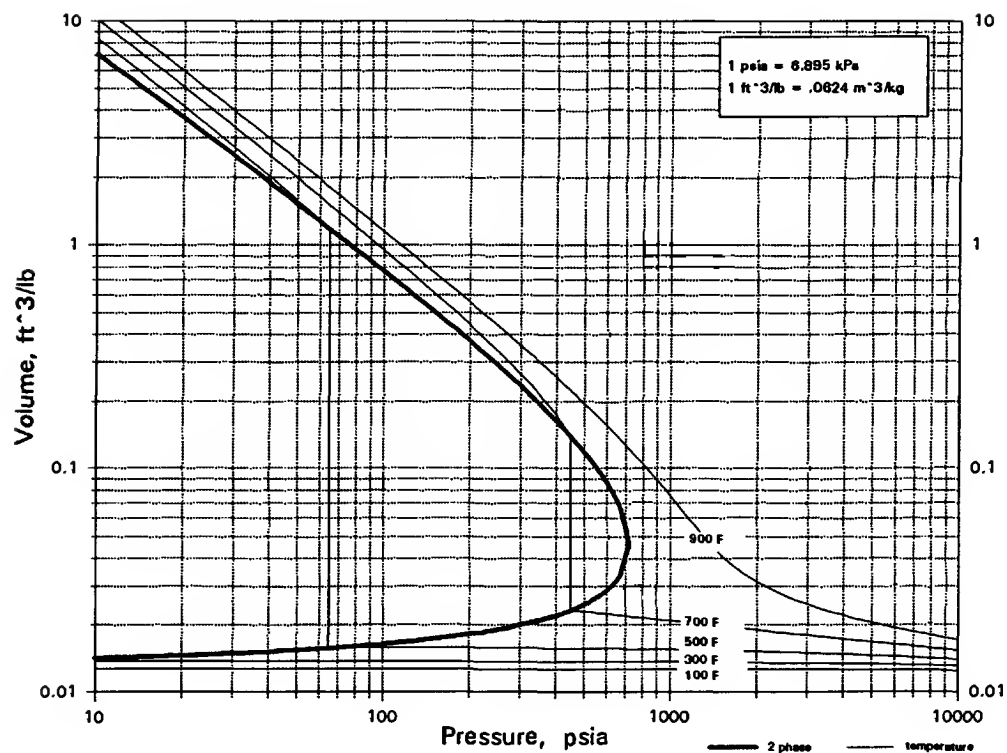
C7H6O2

p-HYDROXYBENZALDEHYDE



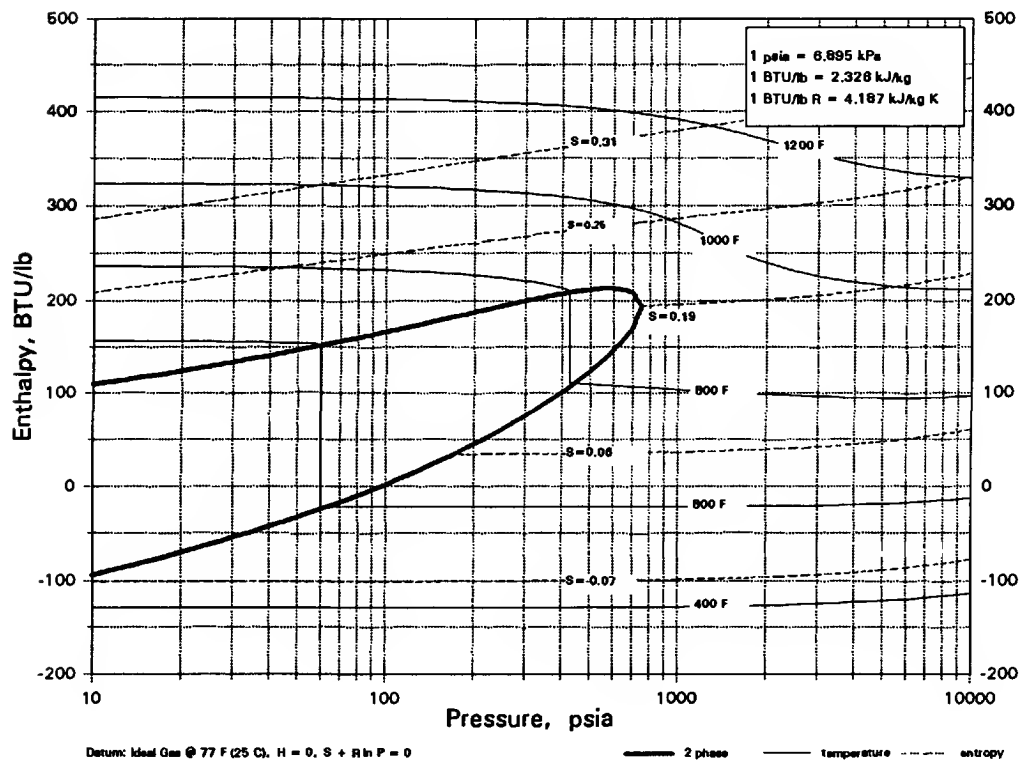
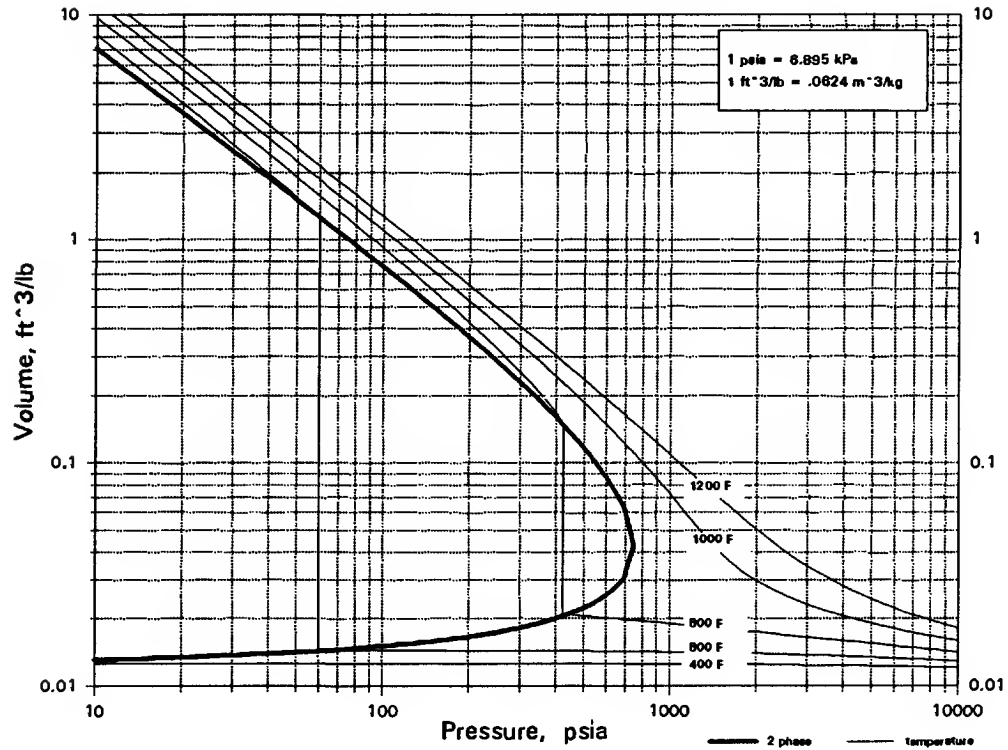
C7H6O2

SALICYLALDEHYDE



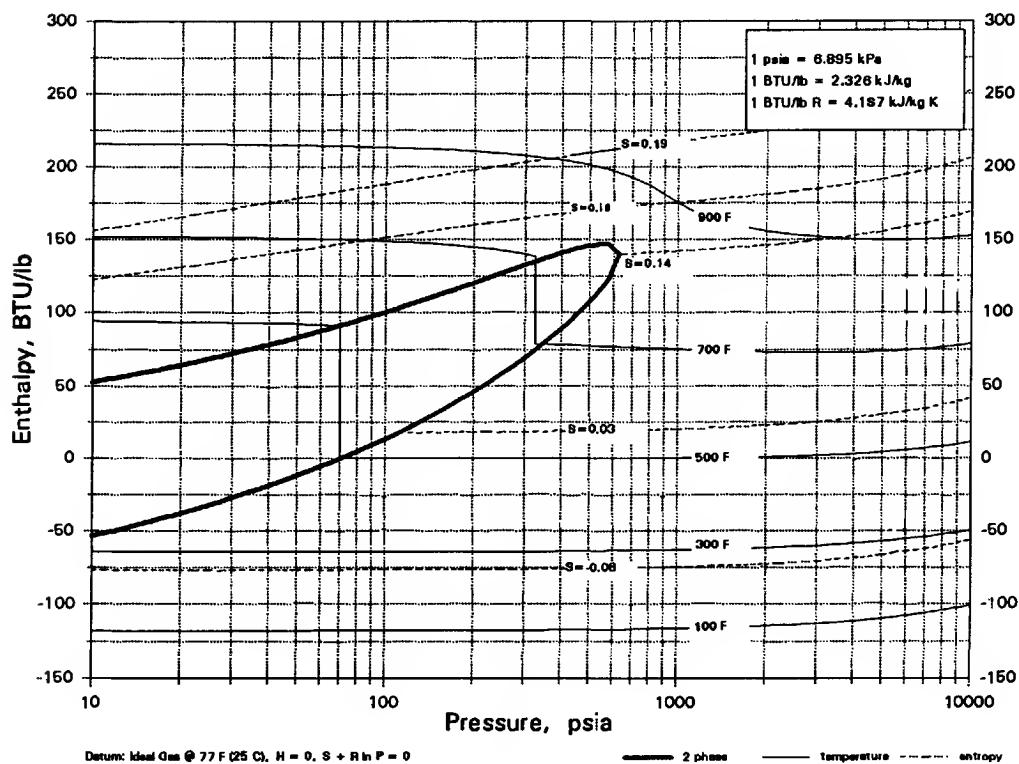
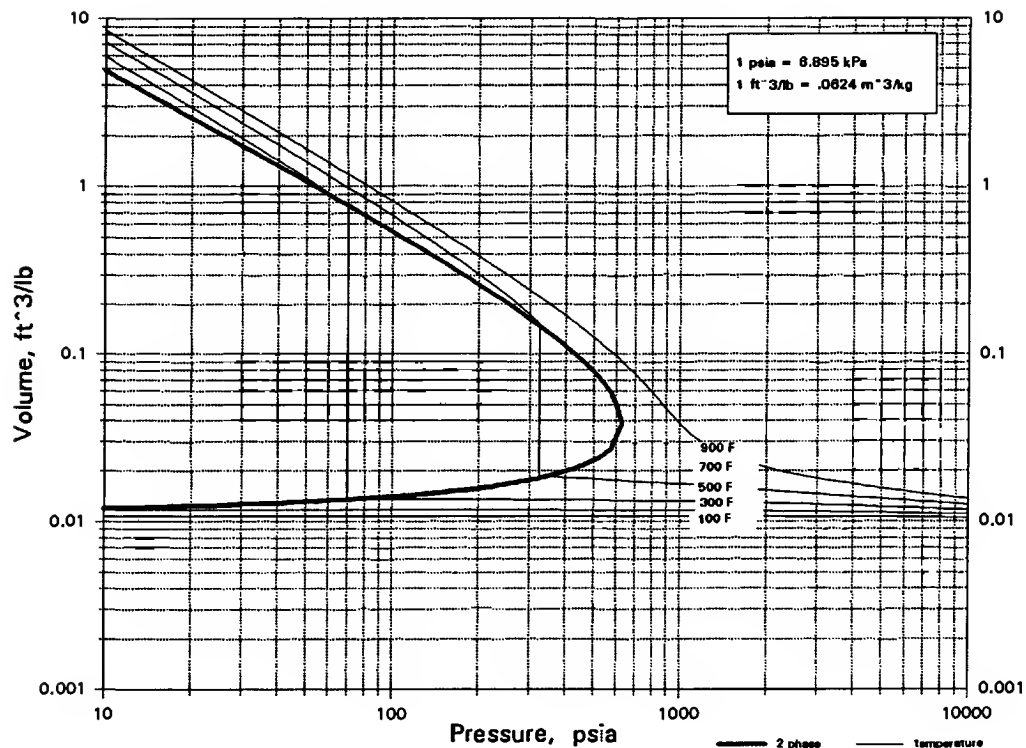
C7H6O3

SALICYLIC ACID



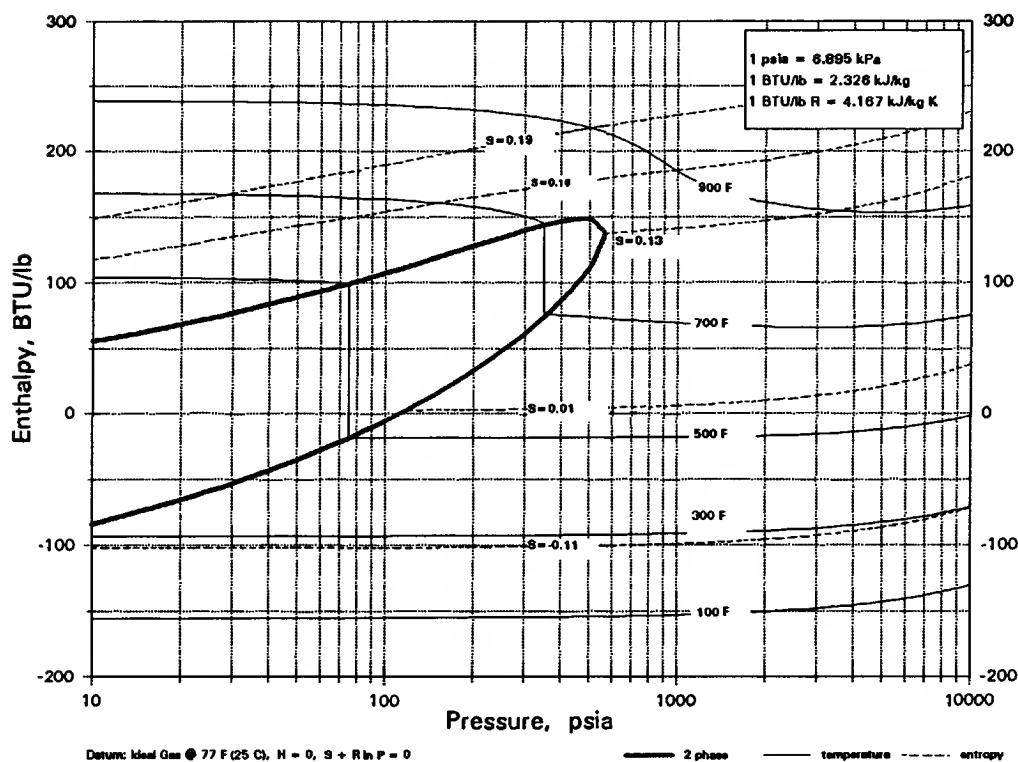
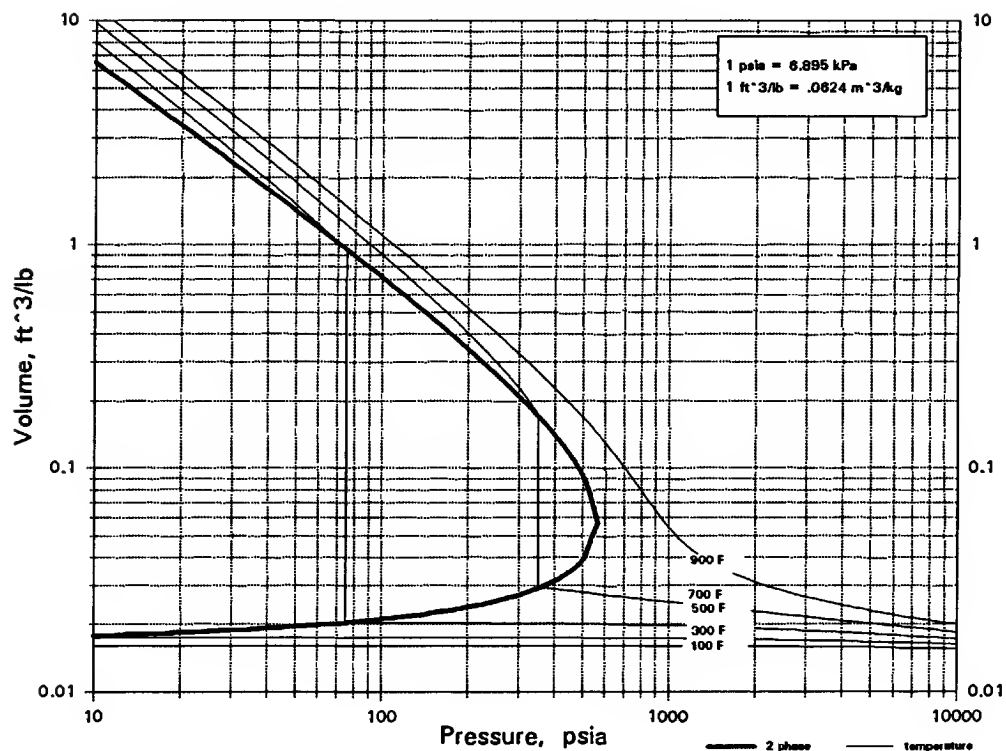
C7H7Br

p-BROMOTOLUENE



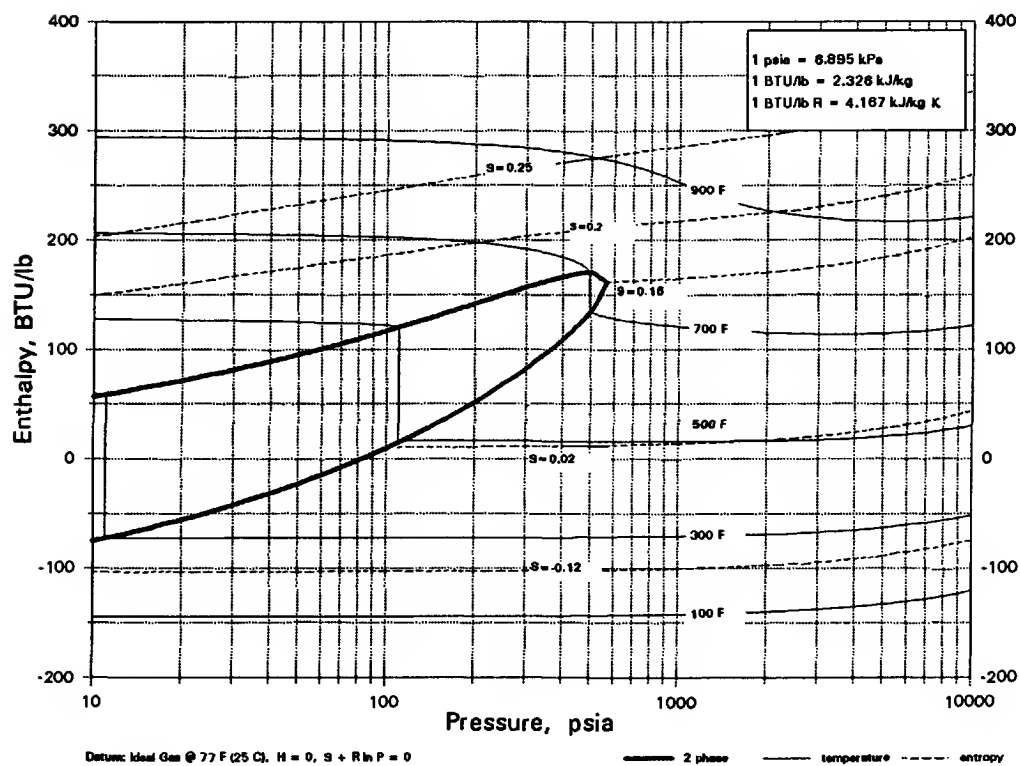
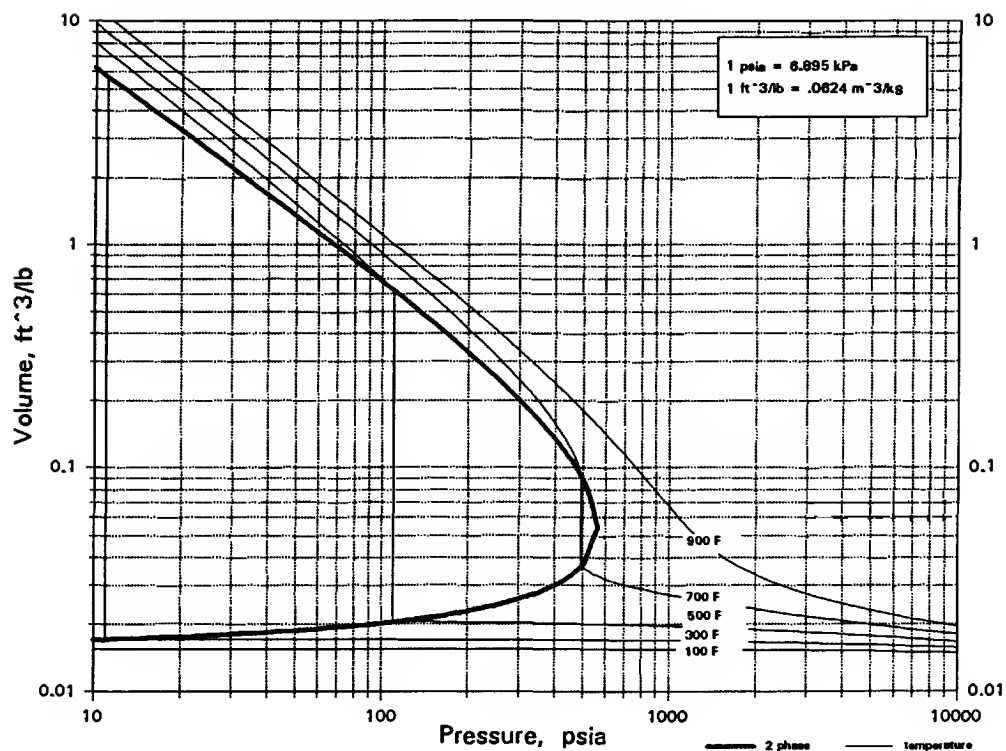
C7H7Cl

BENZYL CHLORIDE



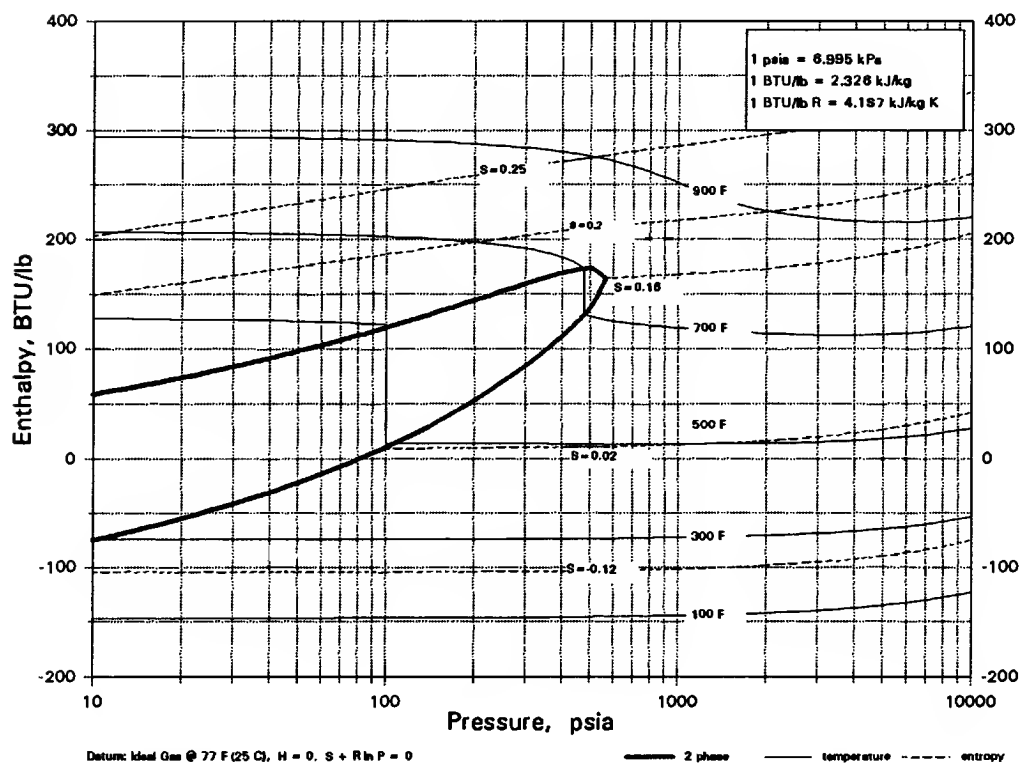
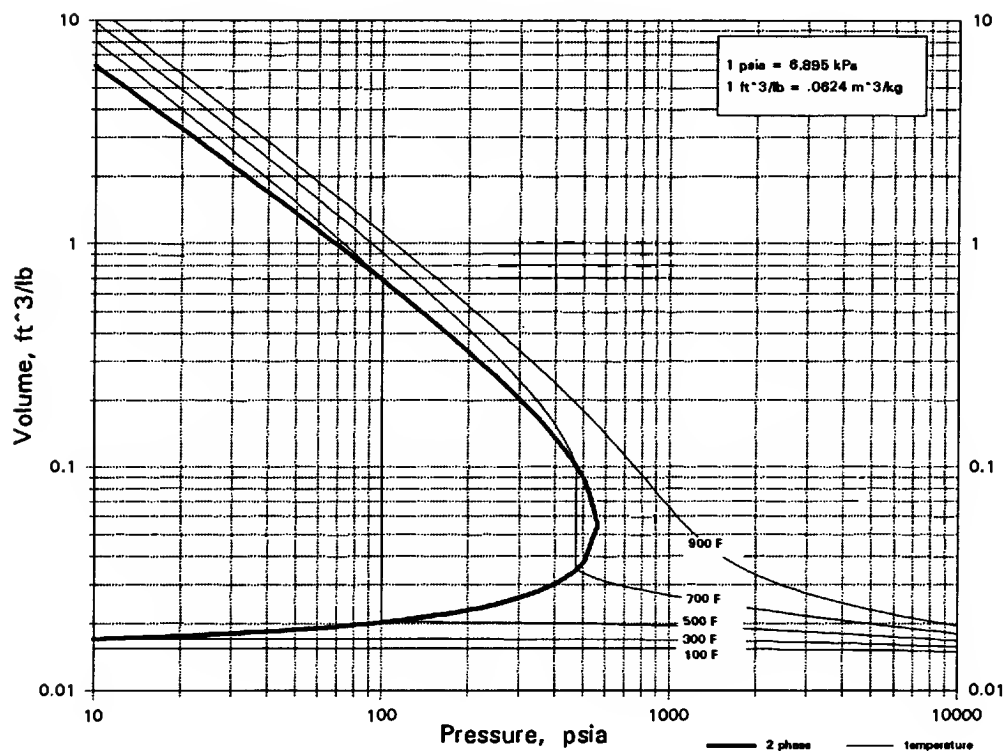
C7H7Cl

o-CHLOROTOLUENE



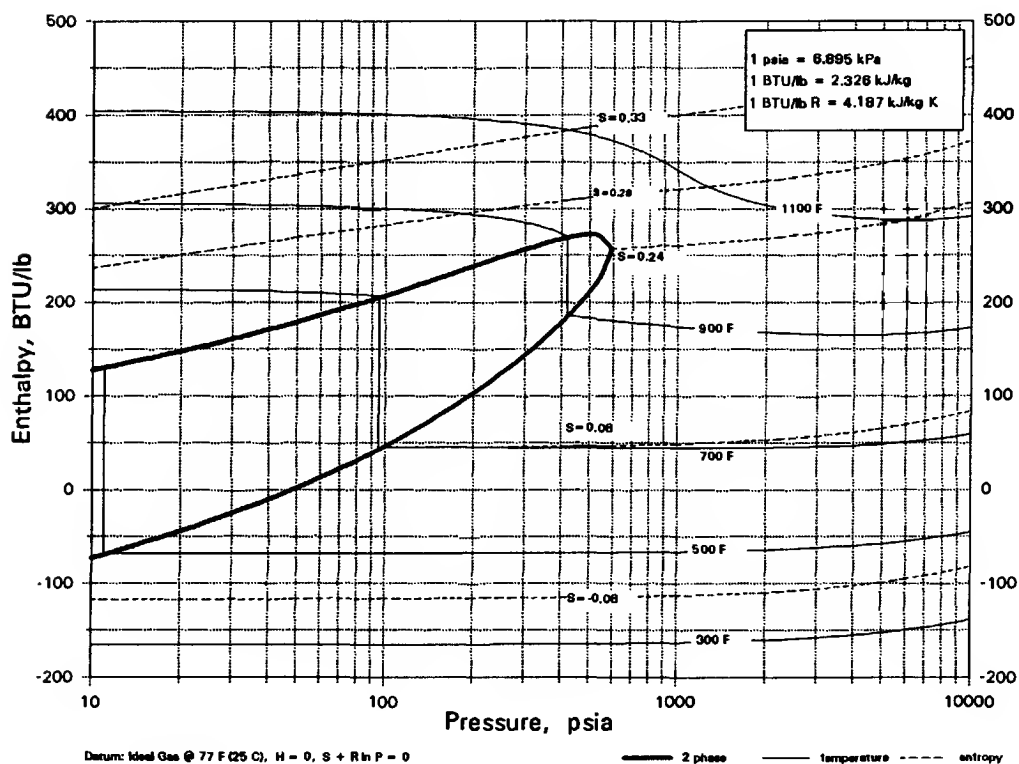
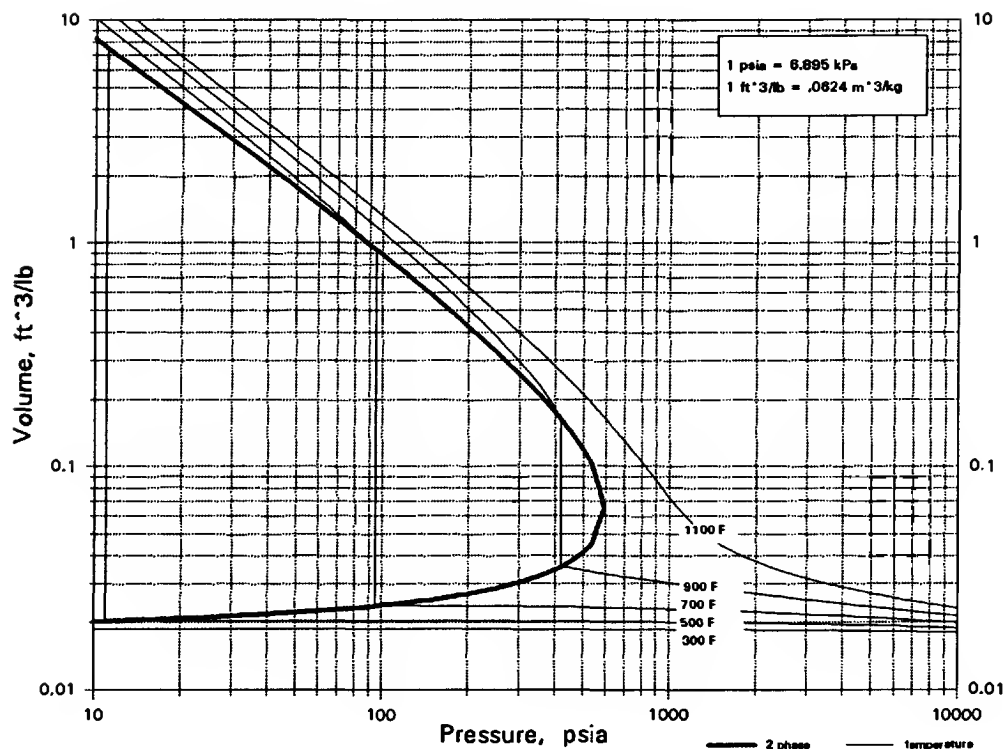
C7H7Cl

p-CHLOROTOLUENE

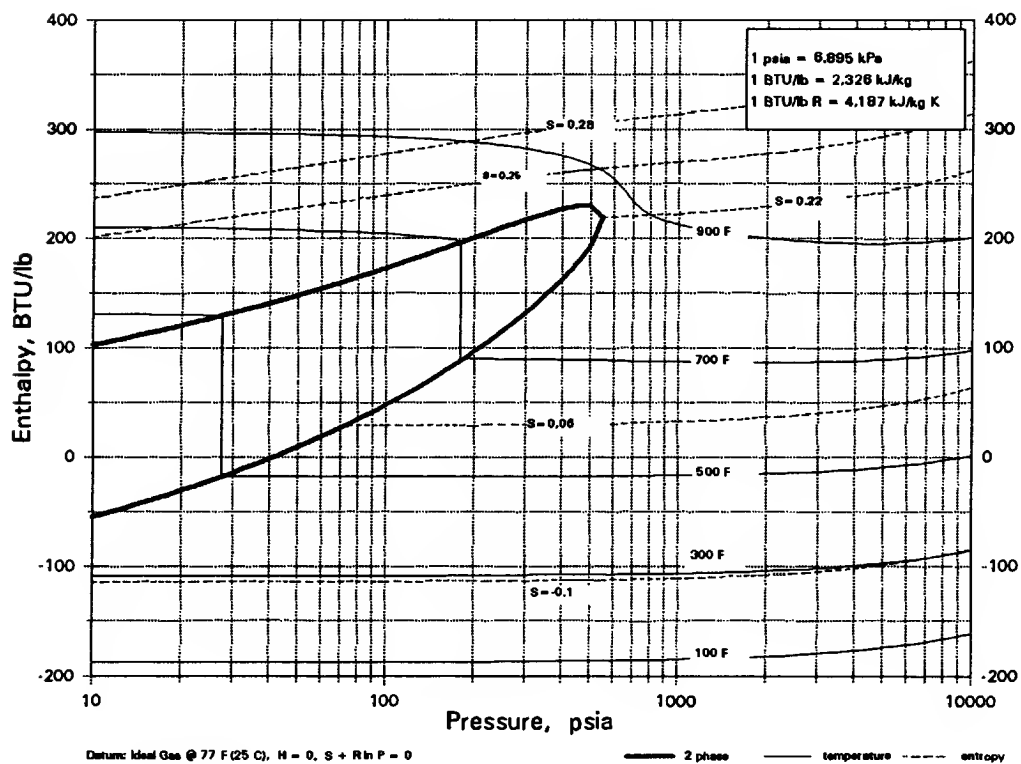
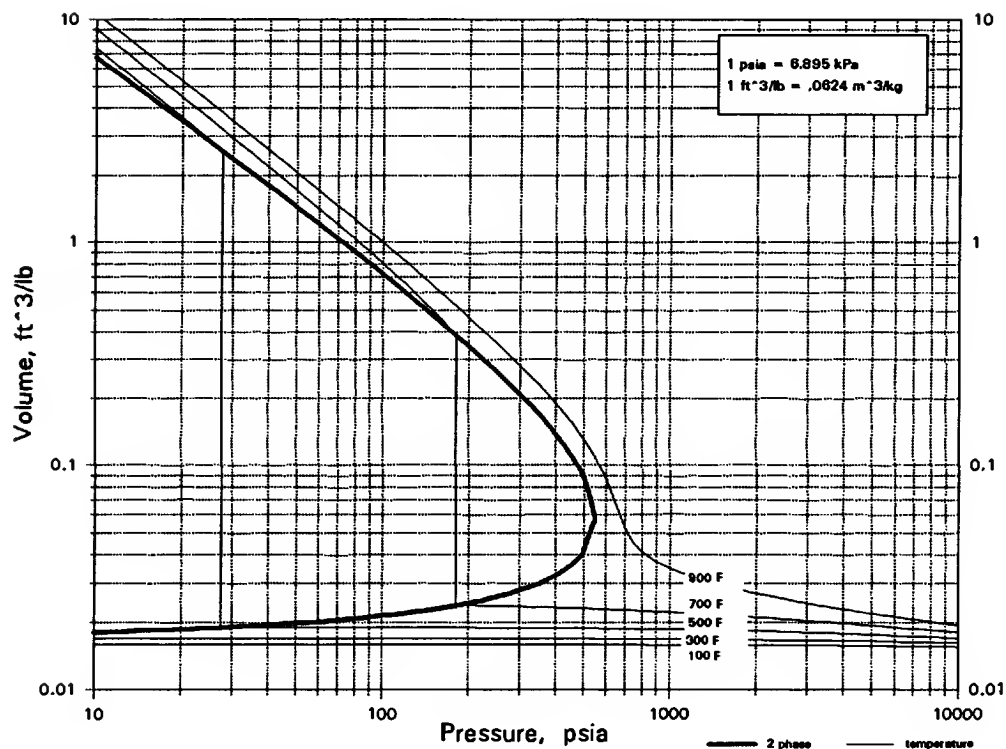


C7H7NO

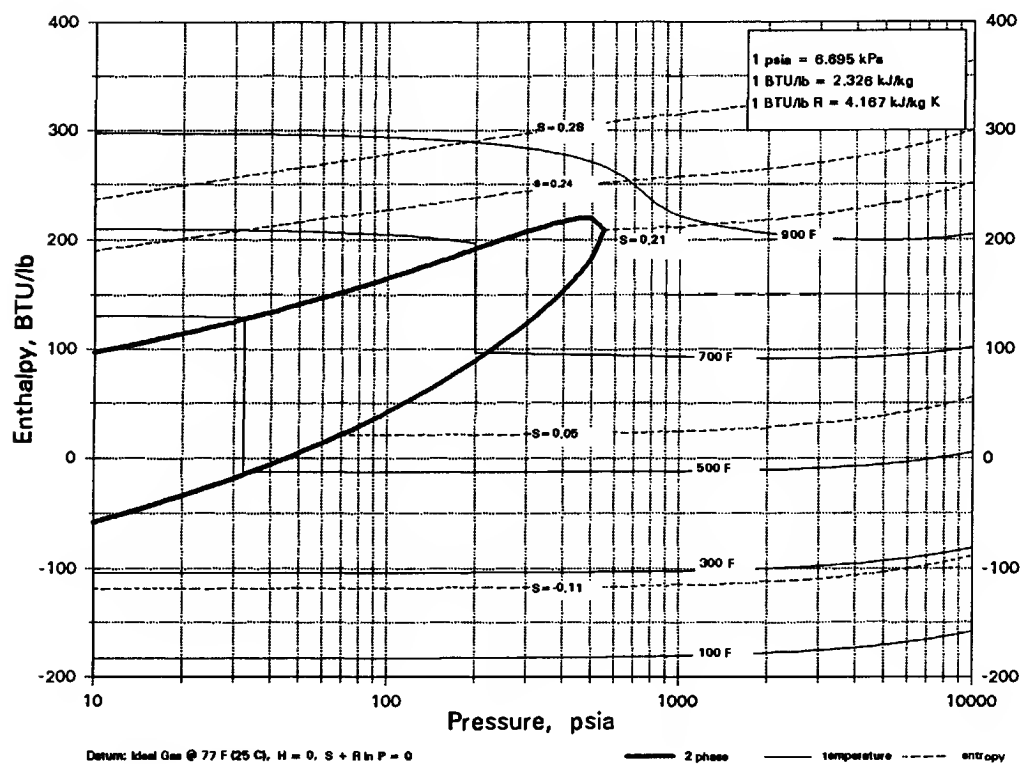
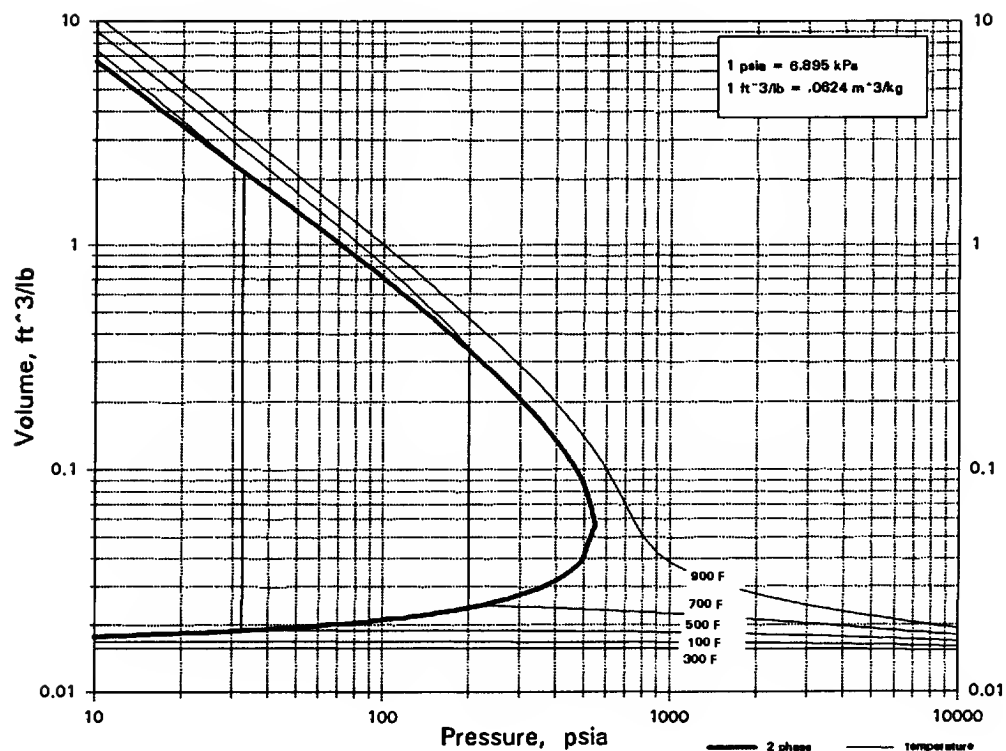
FORMANILIDE



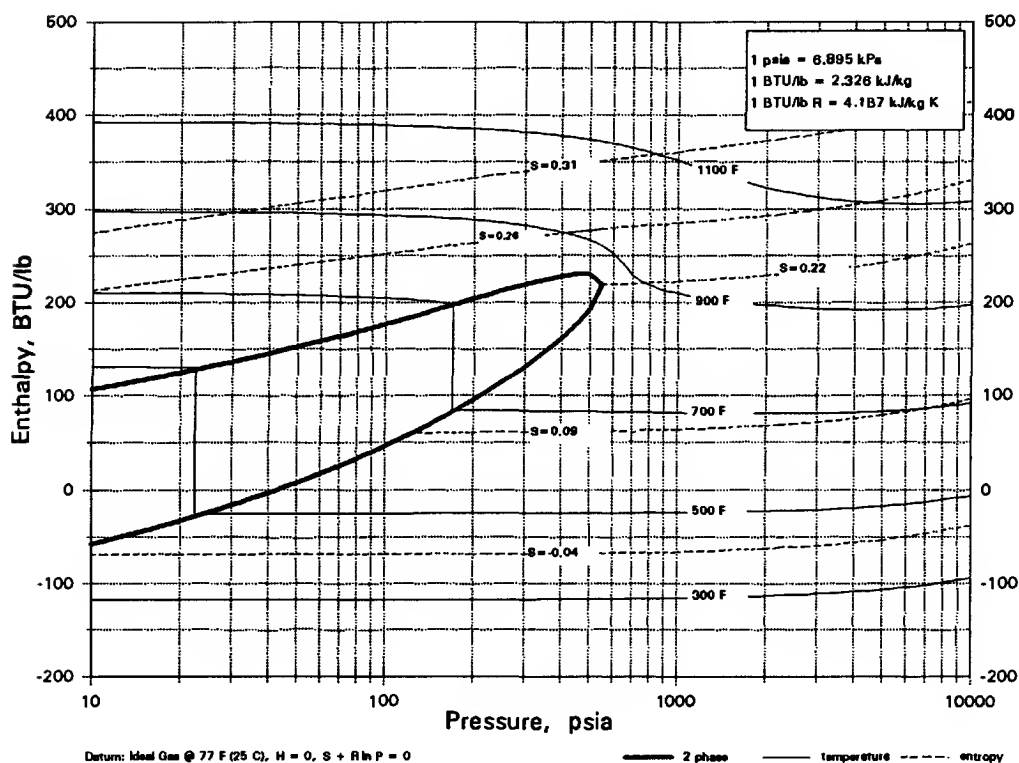
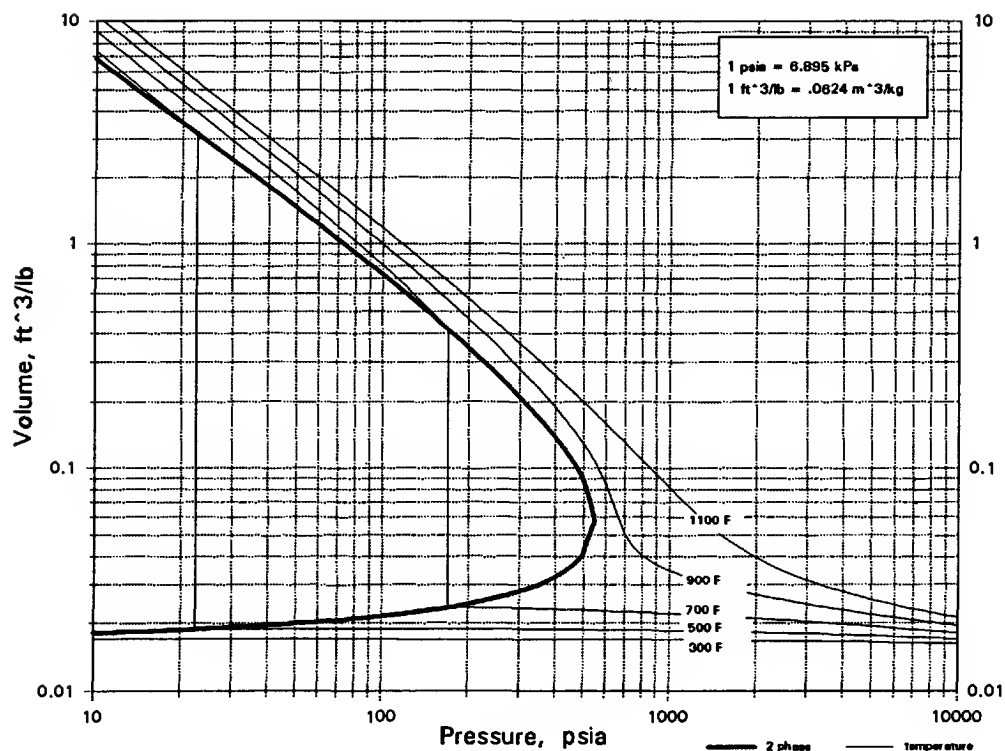
C7H7NO2 m-NITROTOLUENE



C7H7NO2 o-NITROTOLUENE

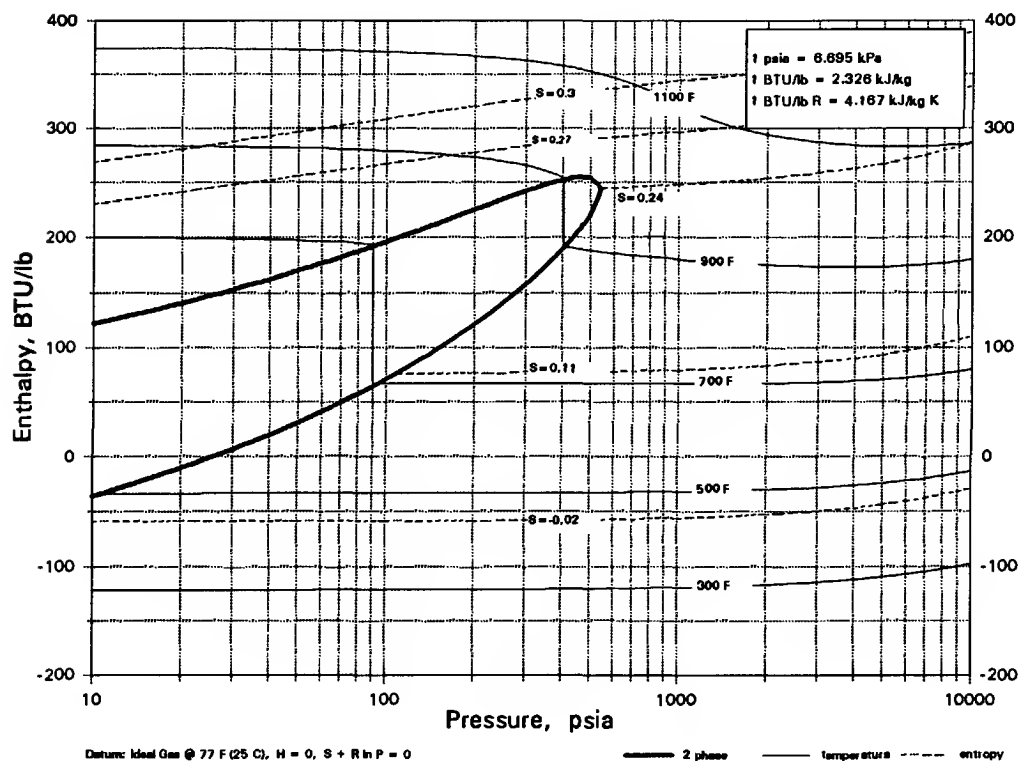
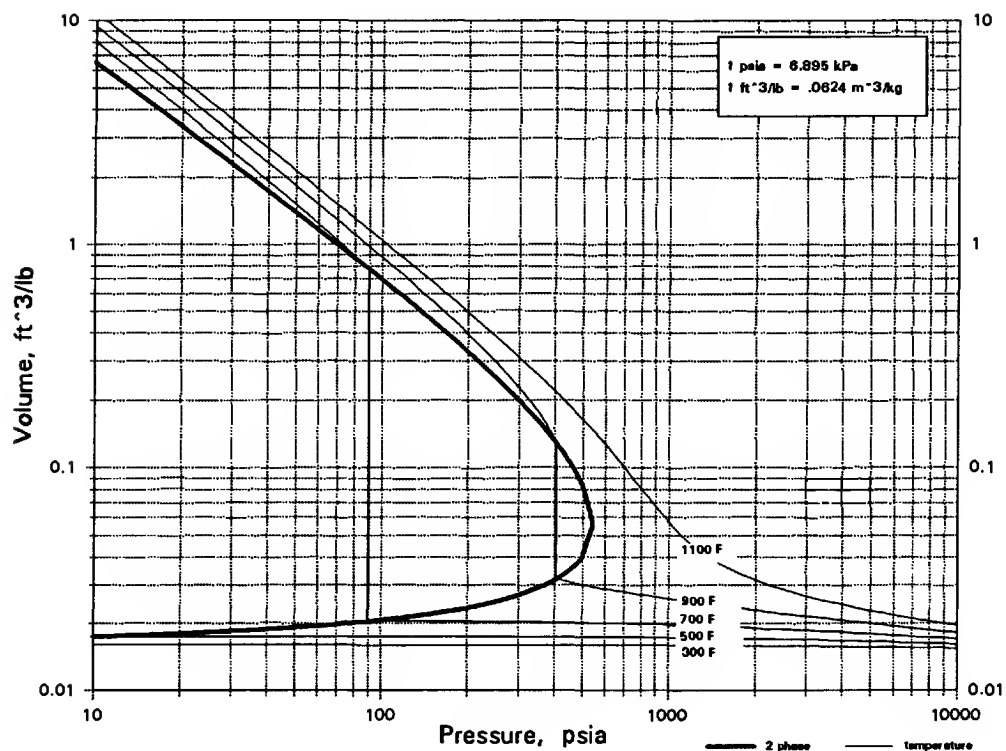


C7H7NO2 p-NITROTOLUENE



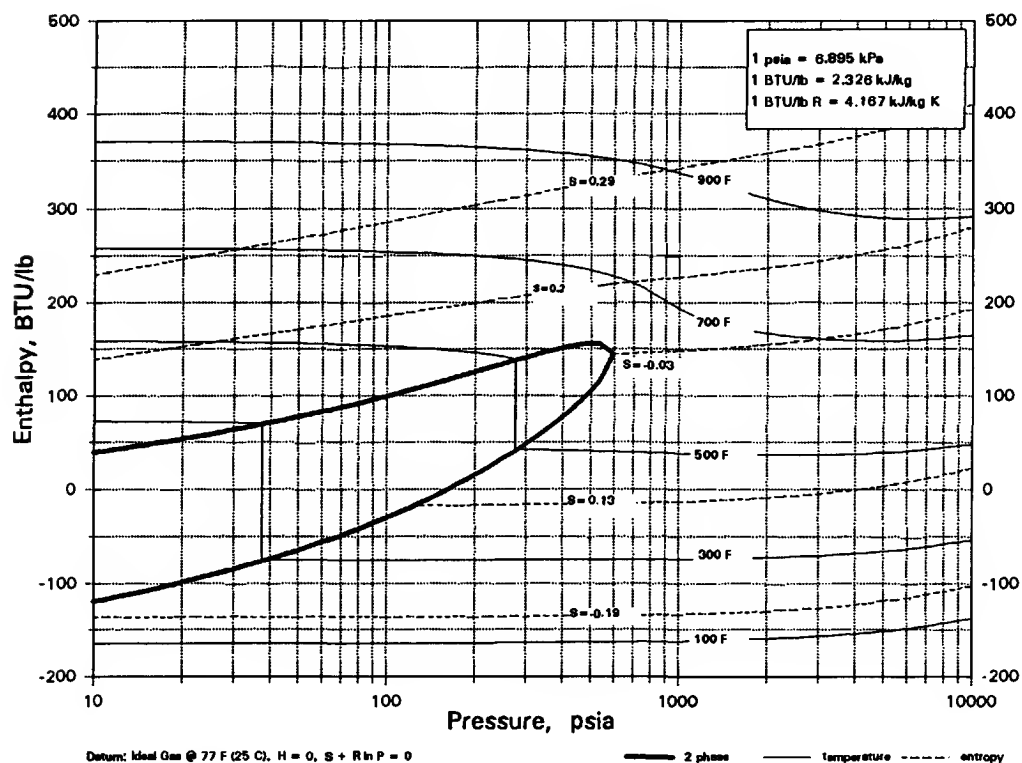
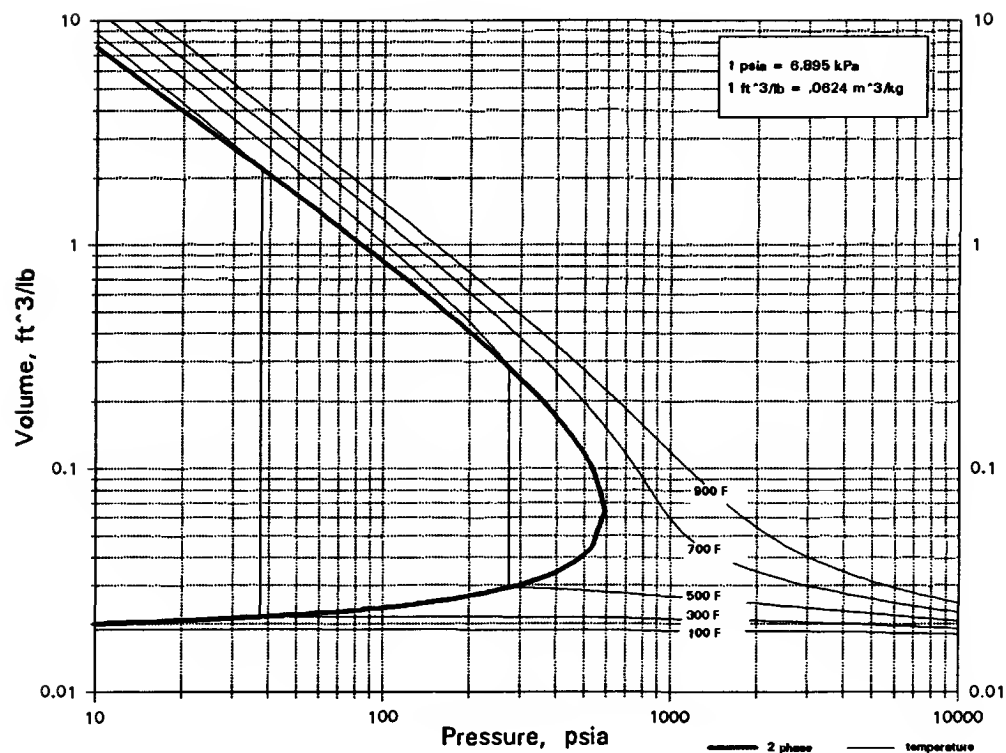
C7H7NO3

o-NITROANISOLE



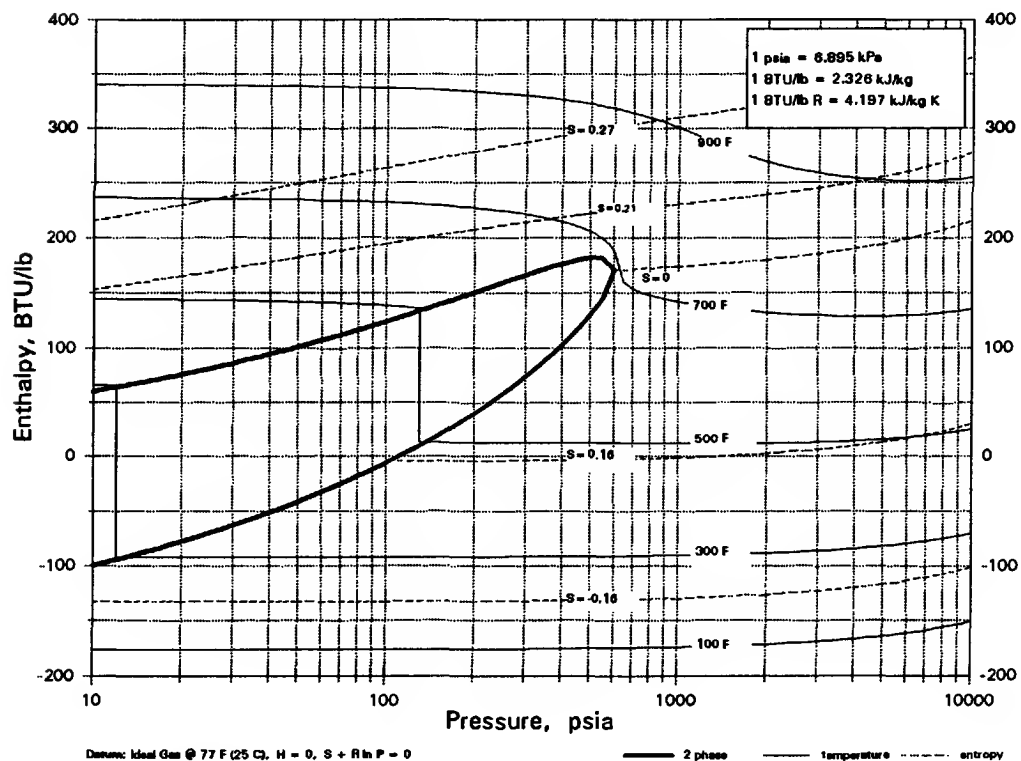
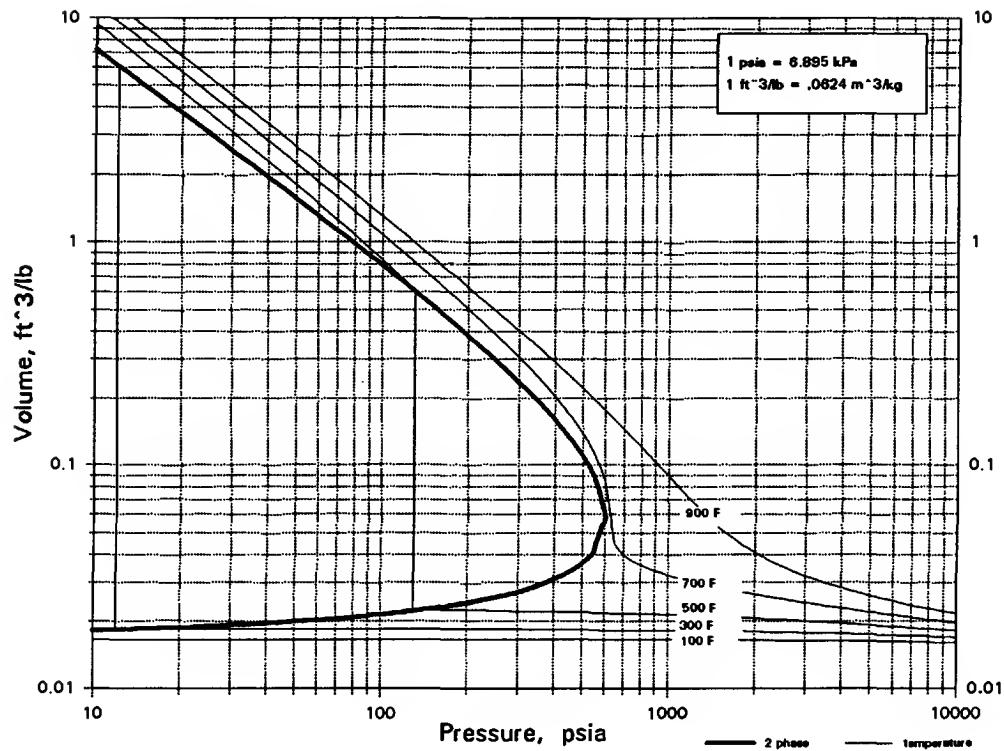
C7H8

TOLUENE



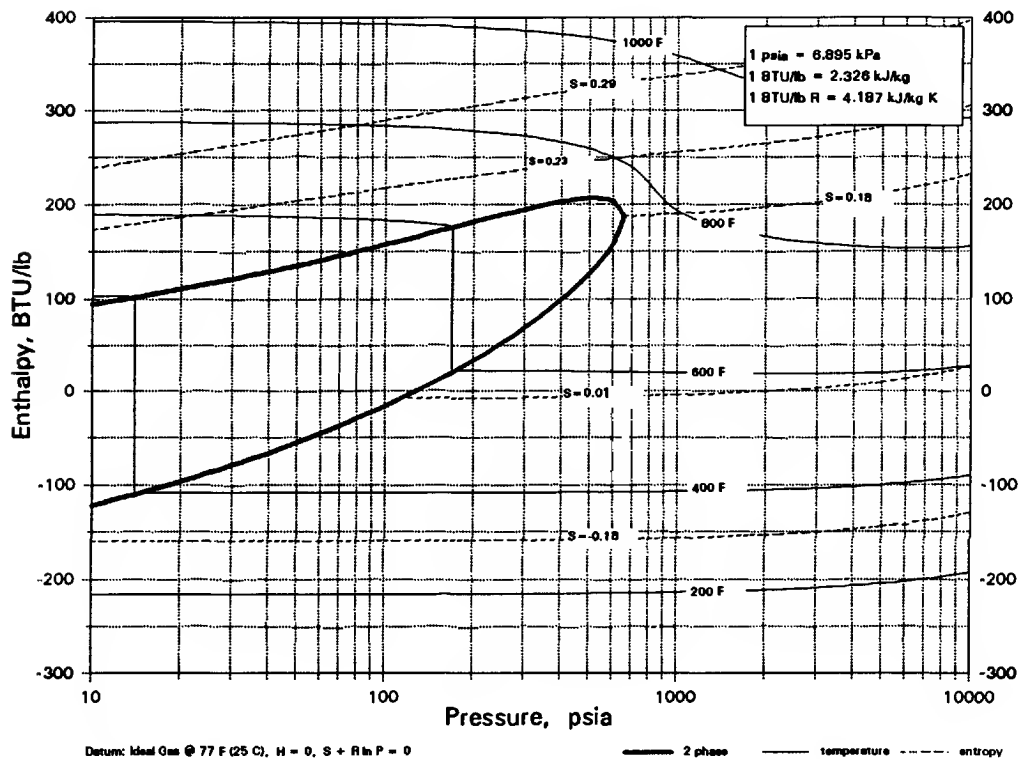
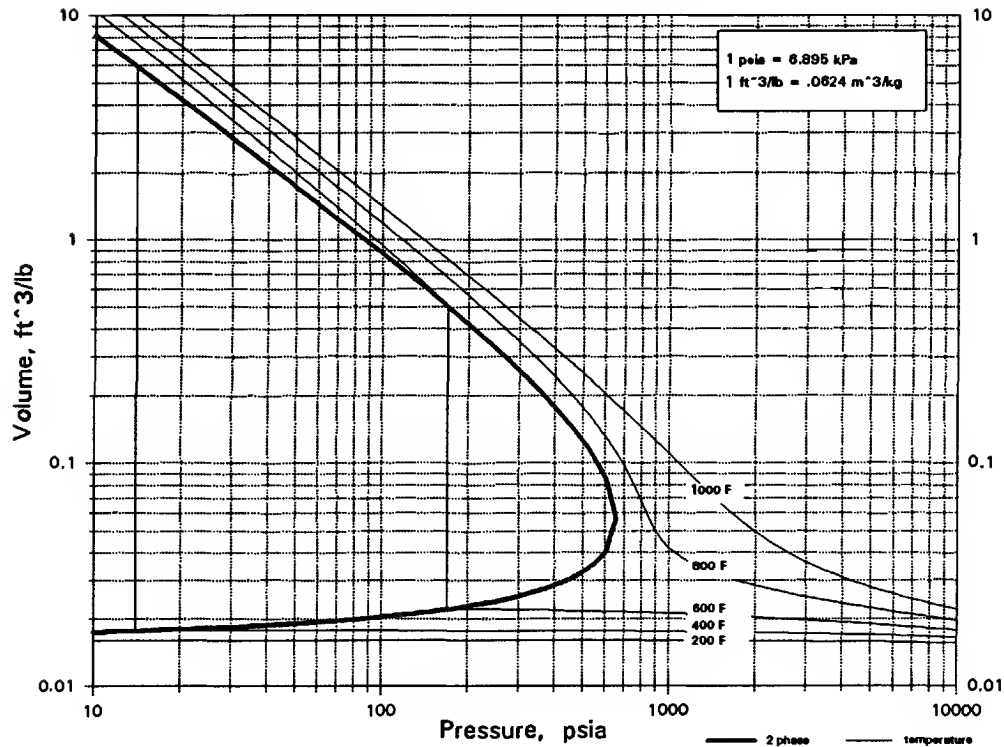
C7H8O

ANISOLE

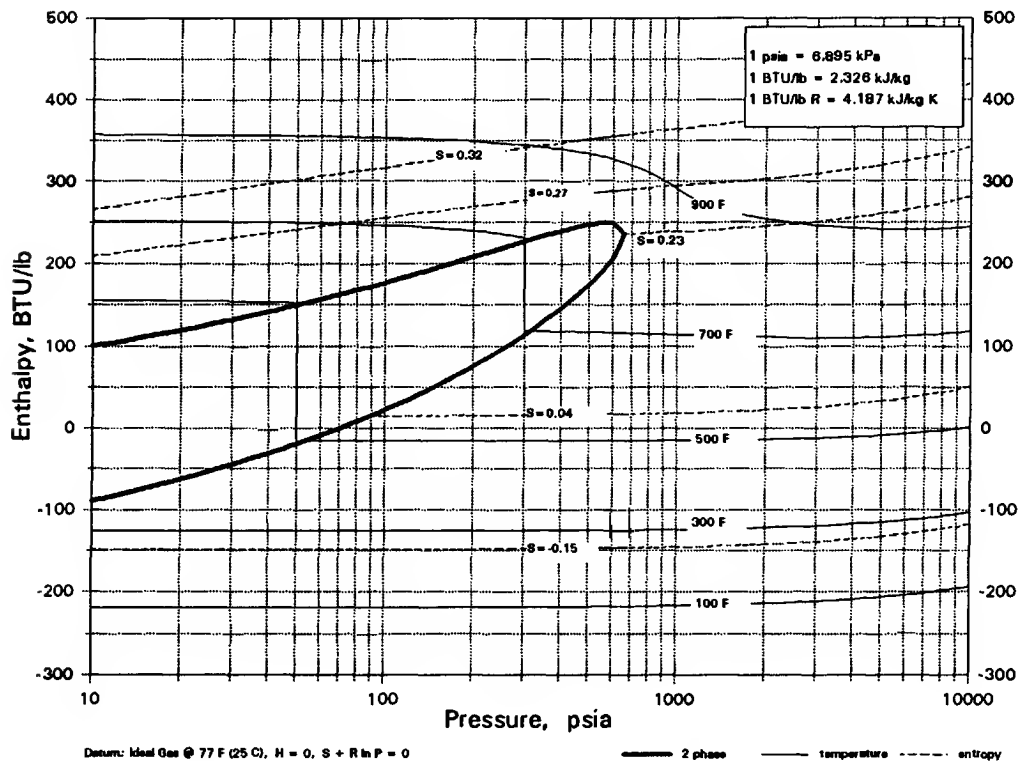
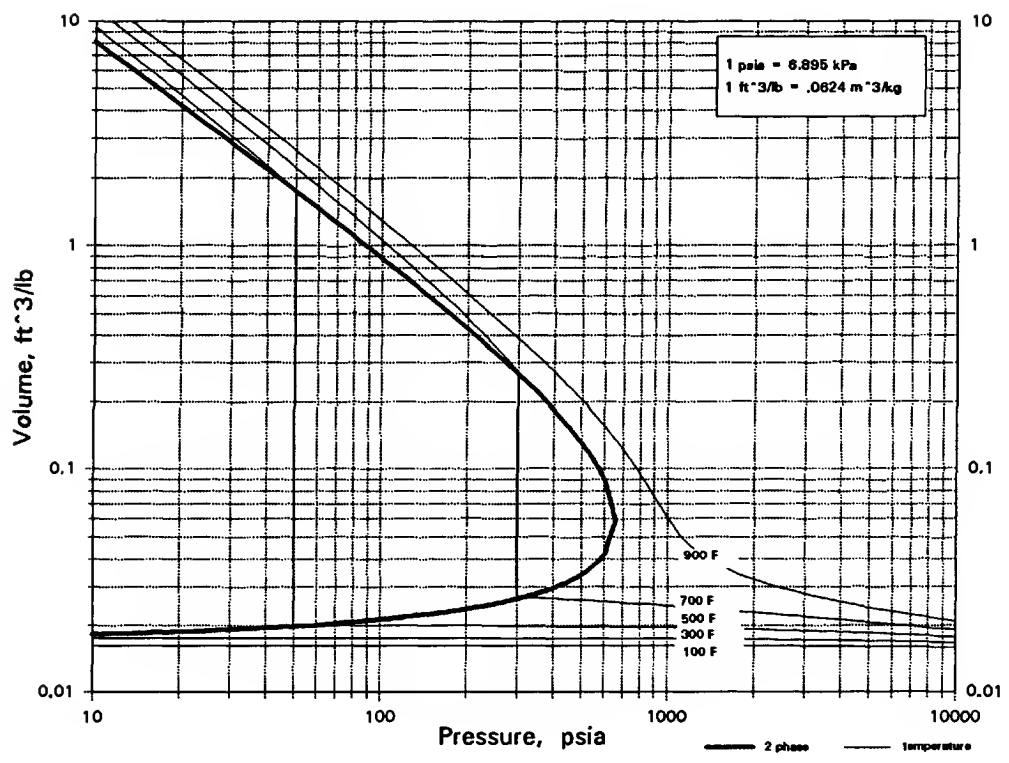


C7H8O

BENZYL ALCOHOL

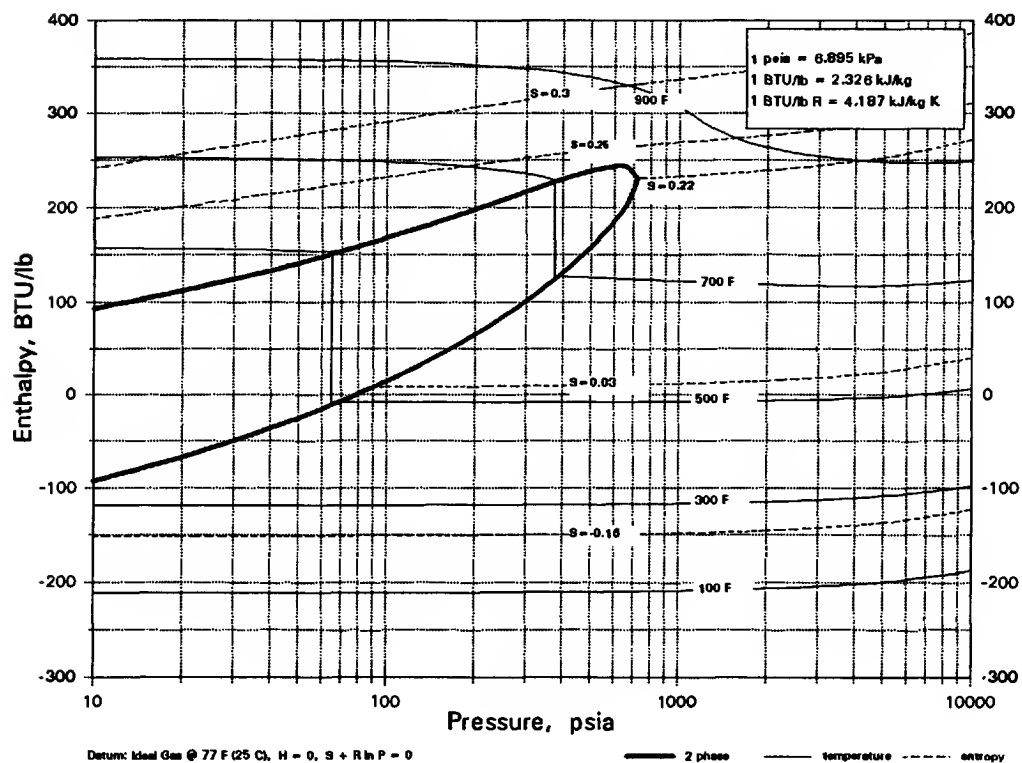
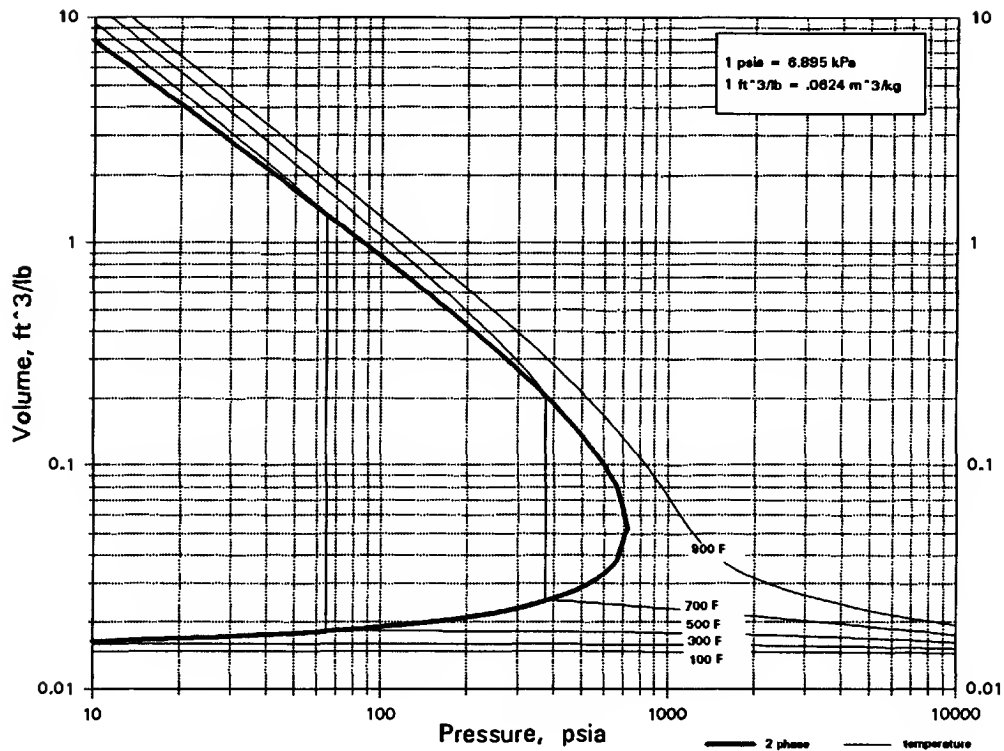


C7H8O
m-CRESOL



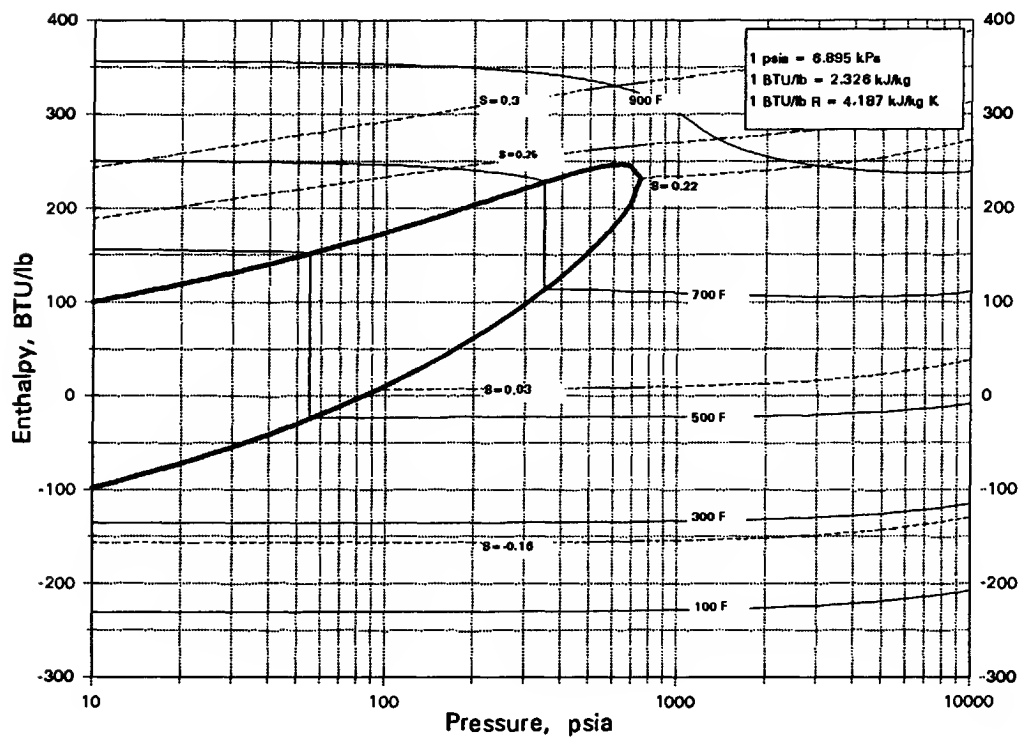
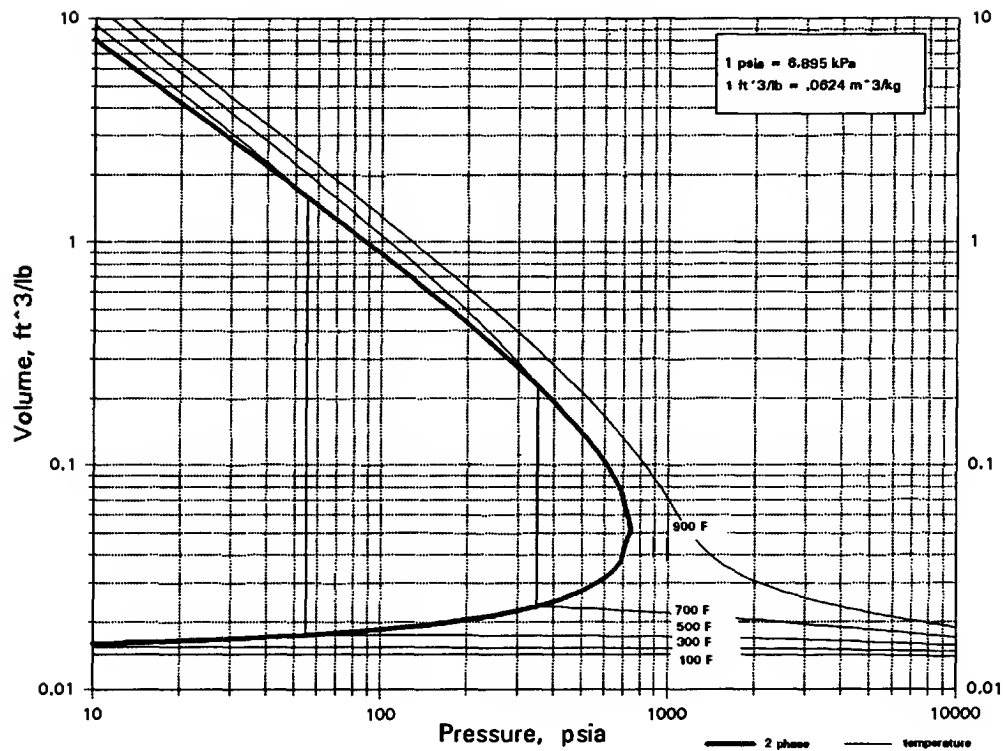
C7H8O

o-CRESOL



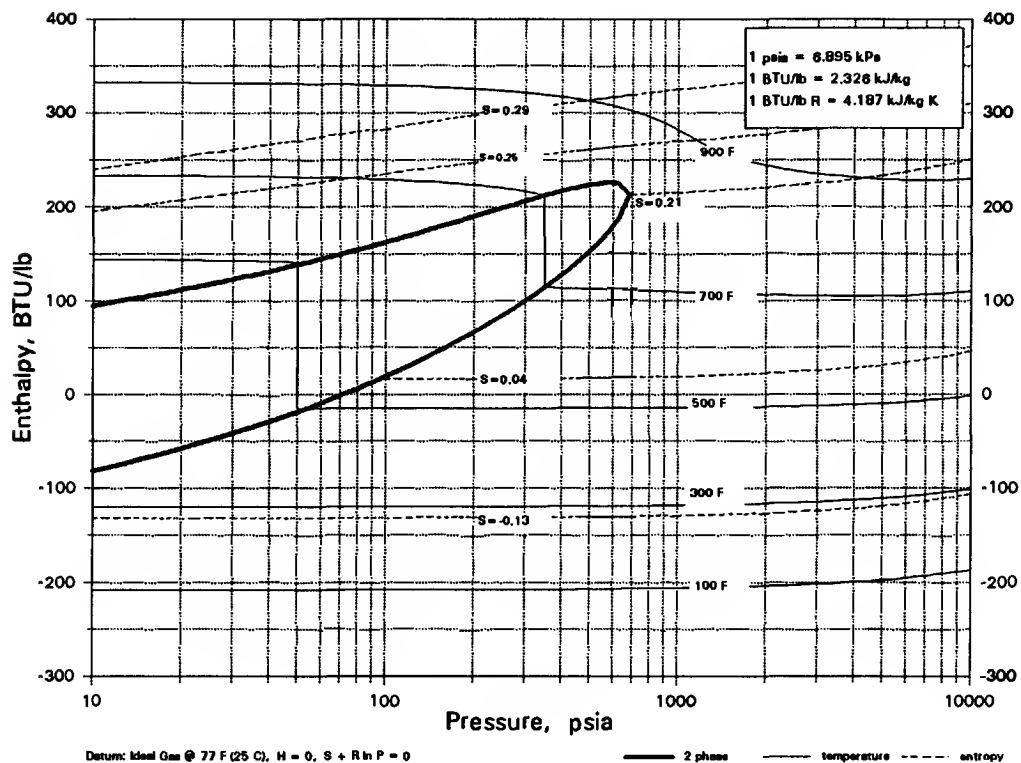
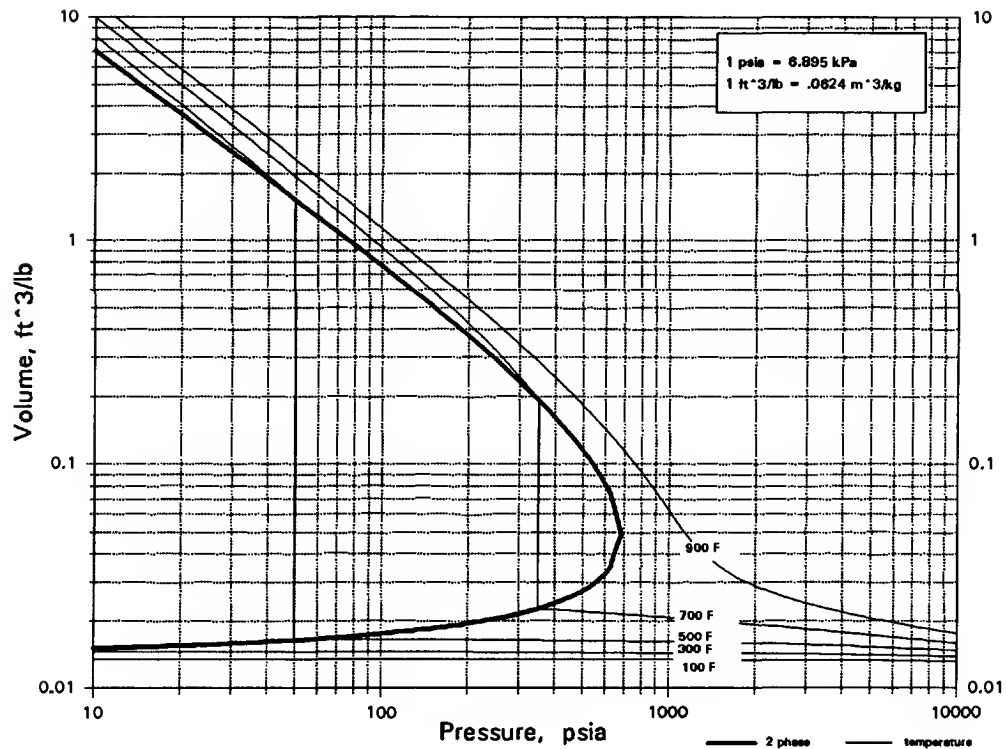
C7H8O

p-CRESOL

Datum: Ideal Gas @ 77 F (25 C), $H = 0$, $S + R \ln P = 0$

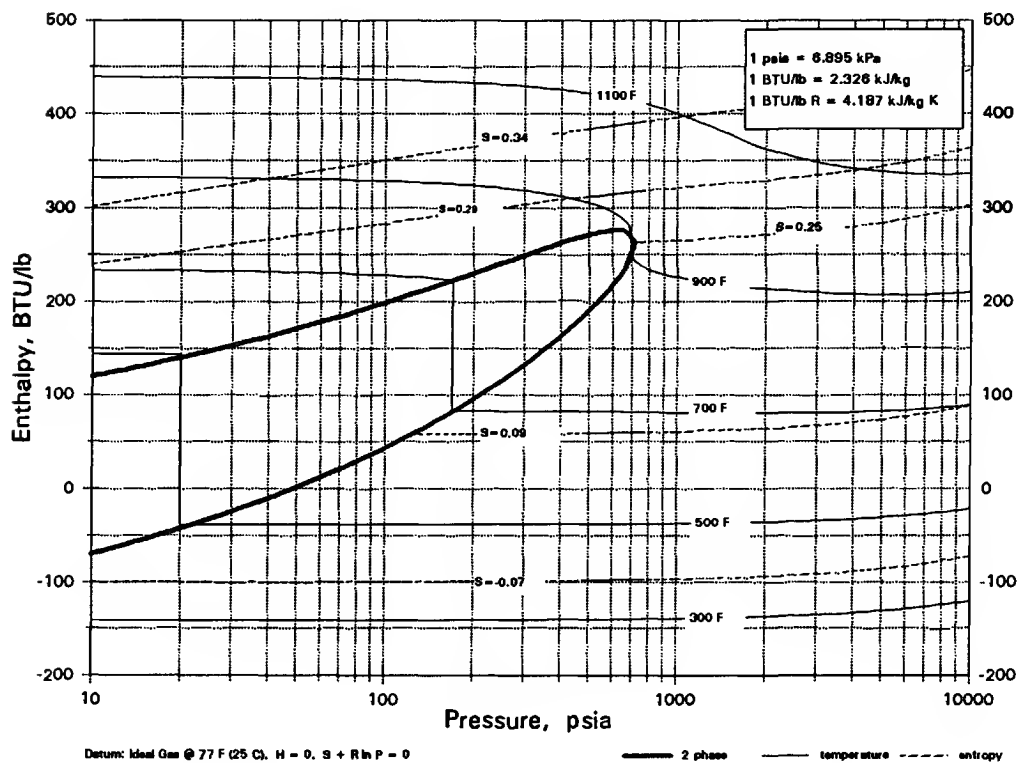
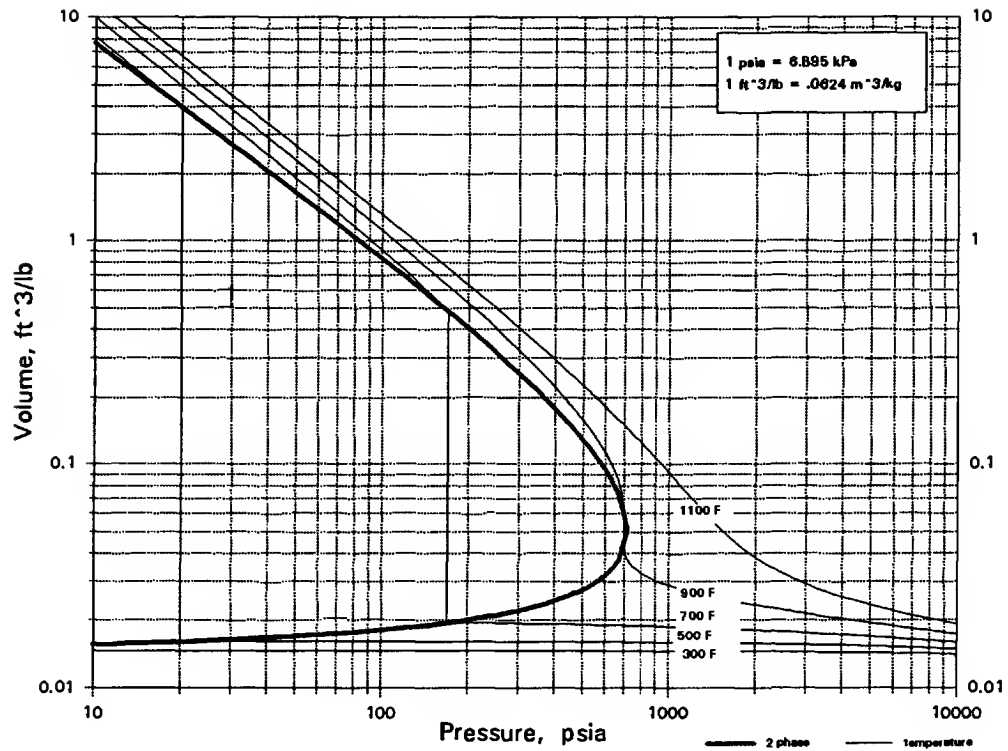
C7H8O2

GUAIACOL



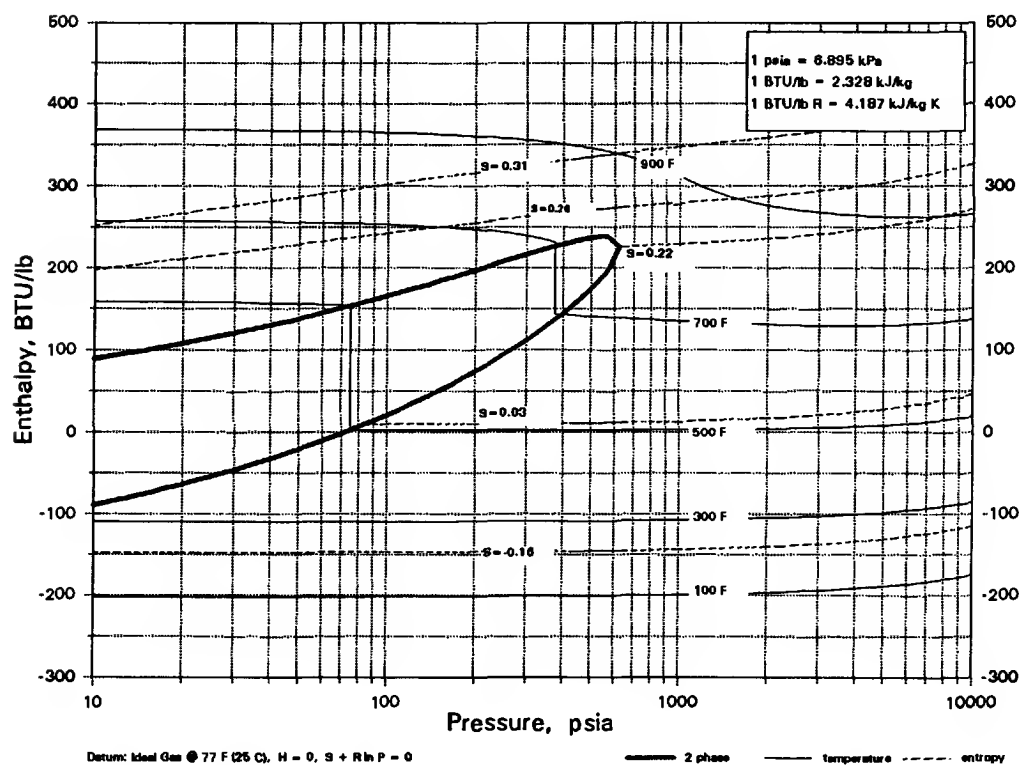
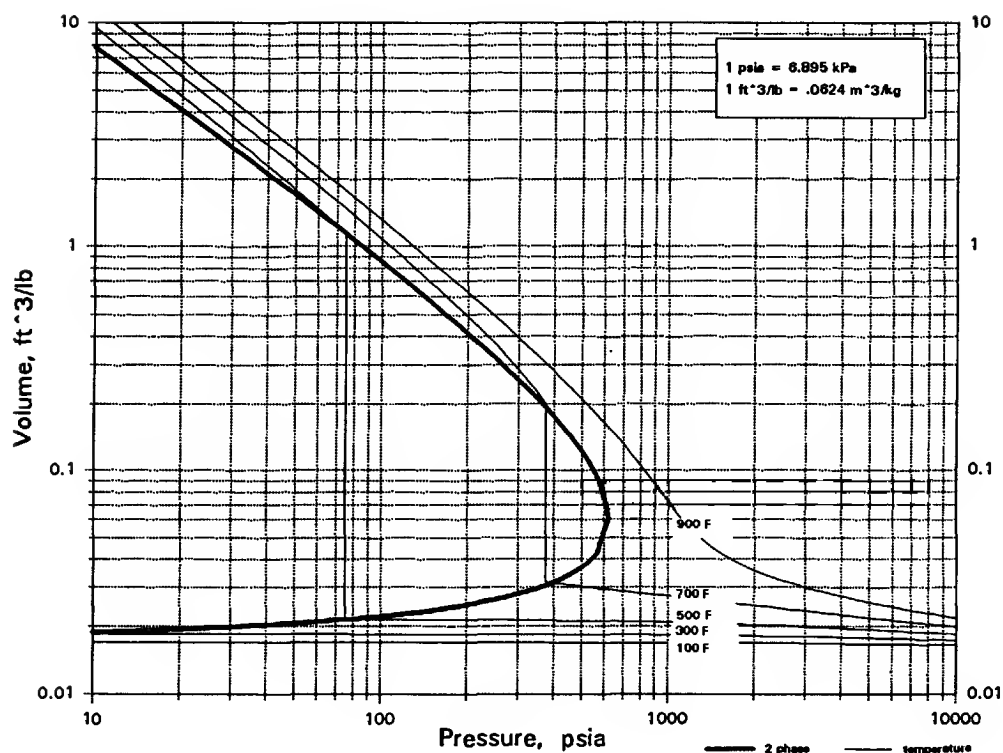
C7H8O2

p-METHOXYPHENOL



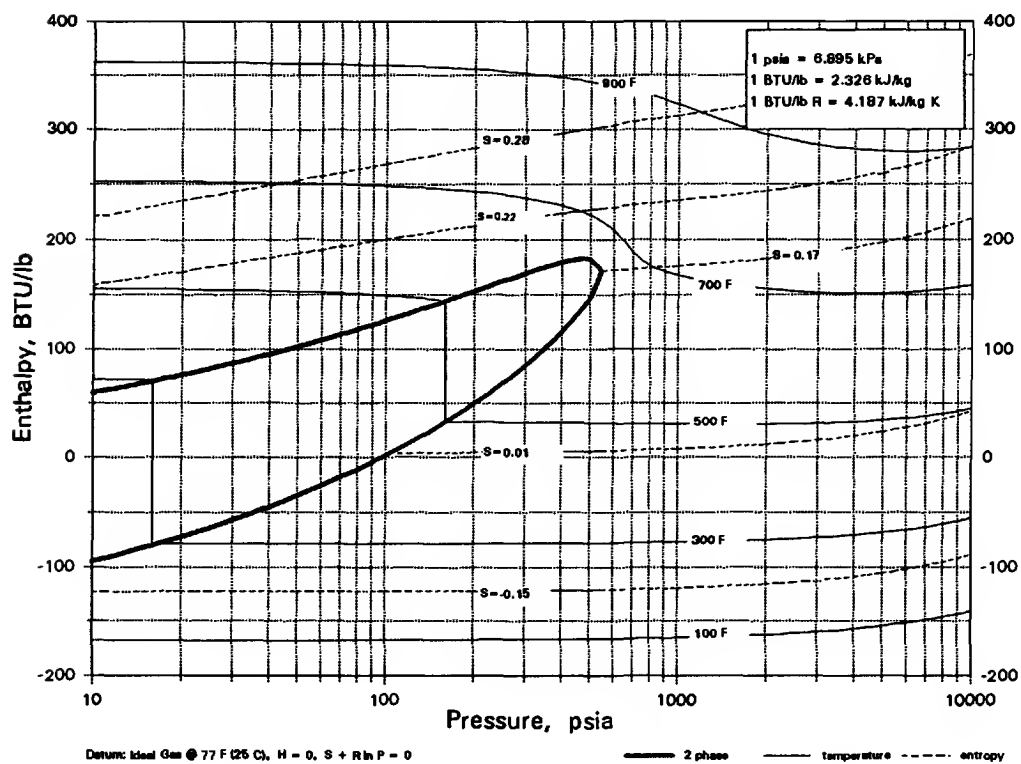
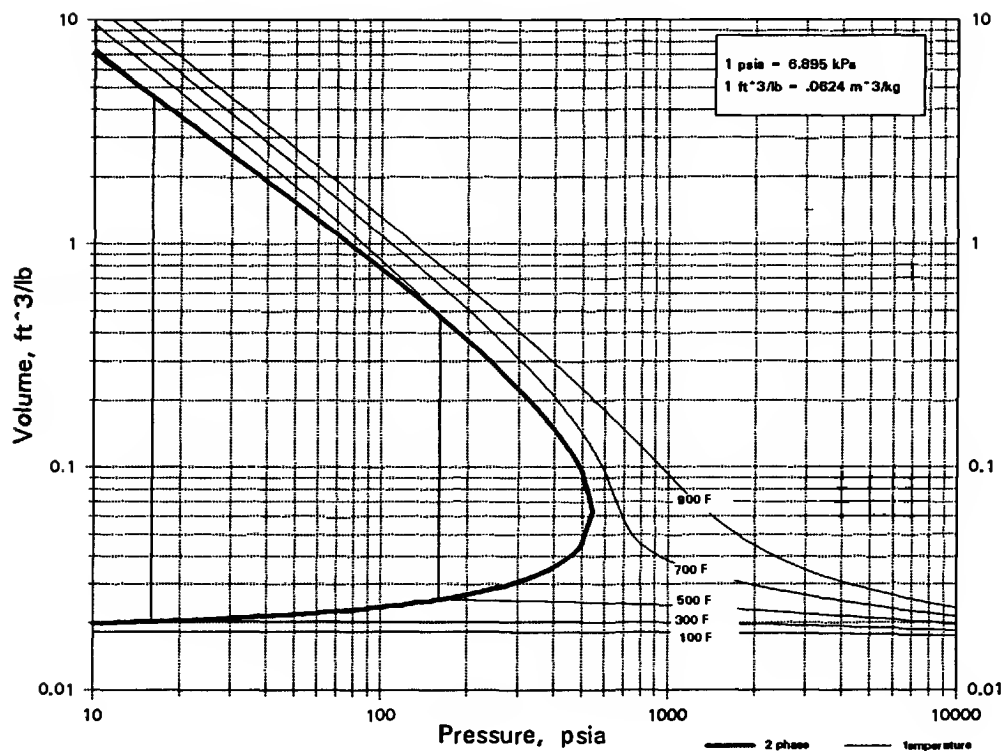
C7H9N

BENZYLAMINE



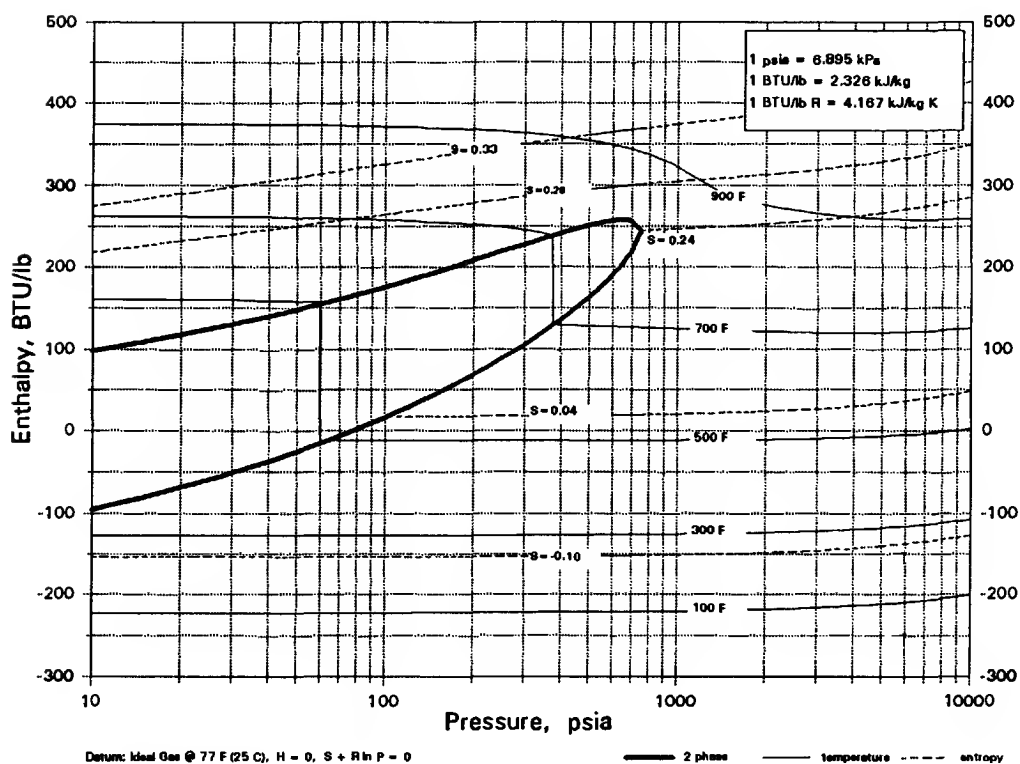
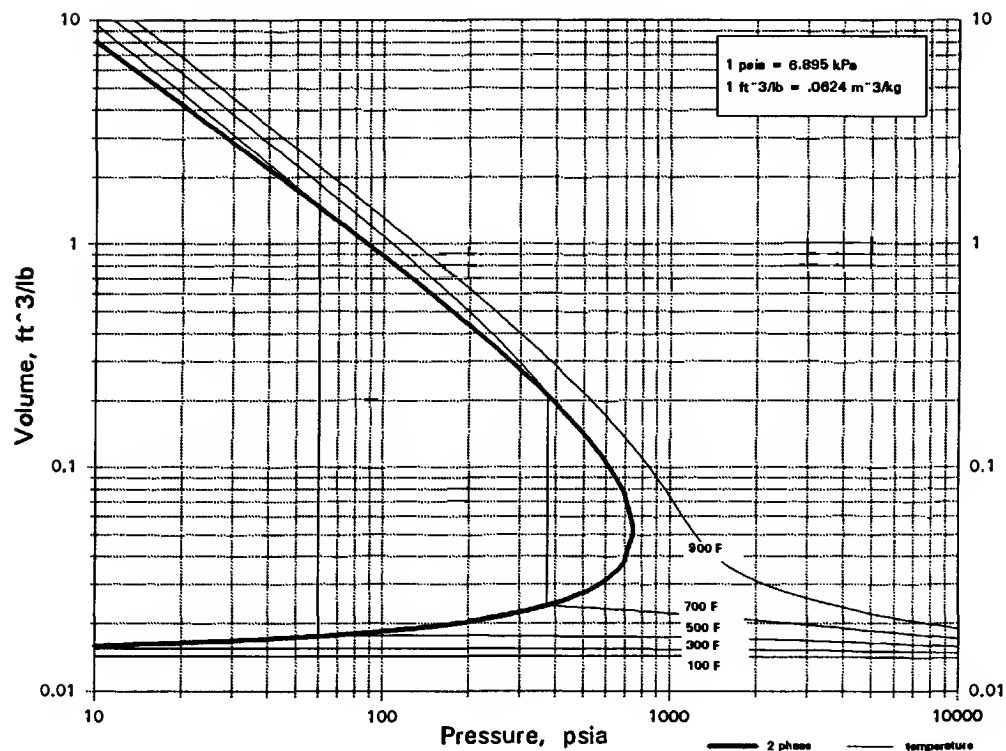
C7H9N

2-6-DIMETHYLPYRIDINE



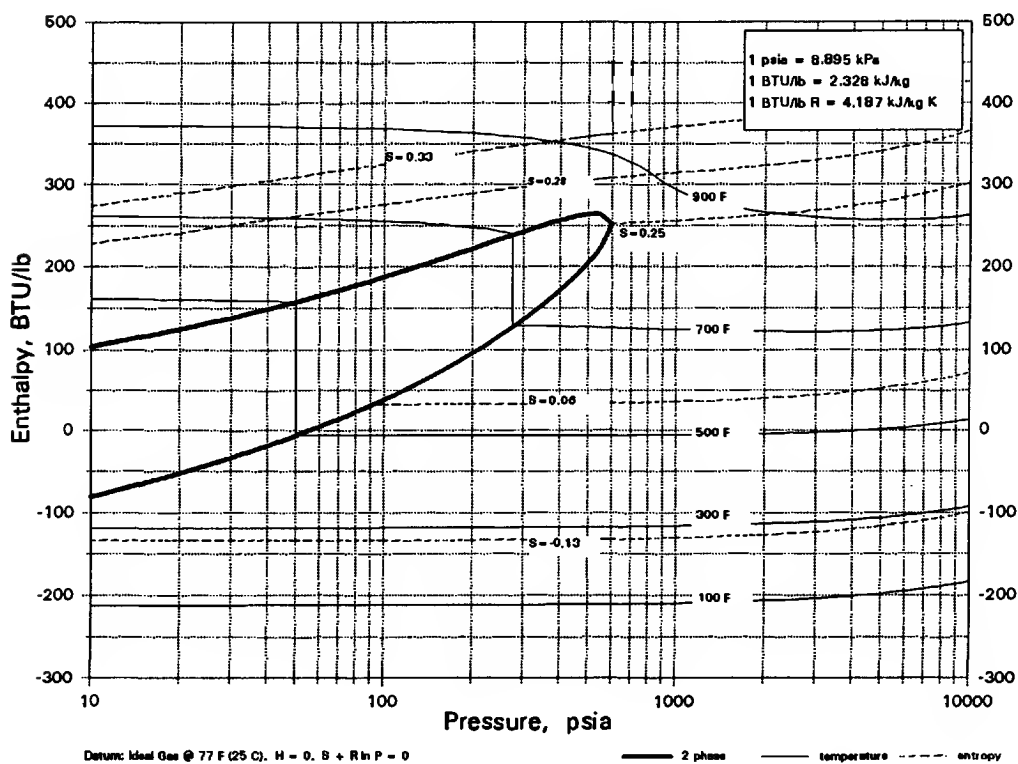
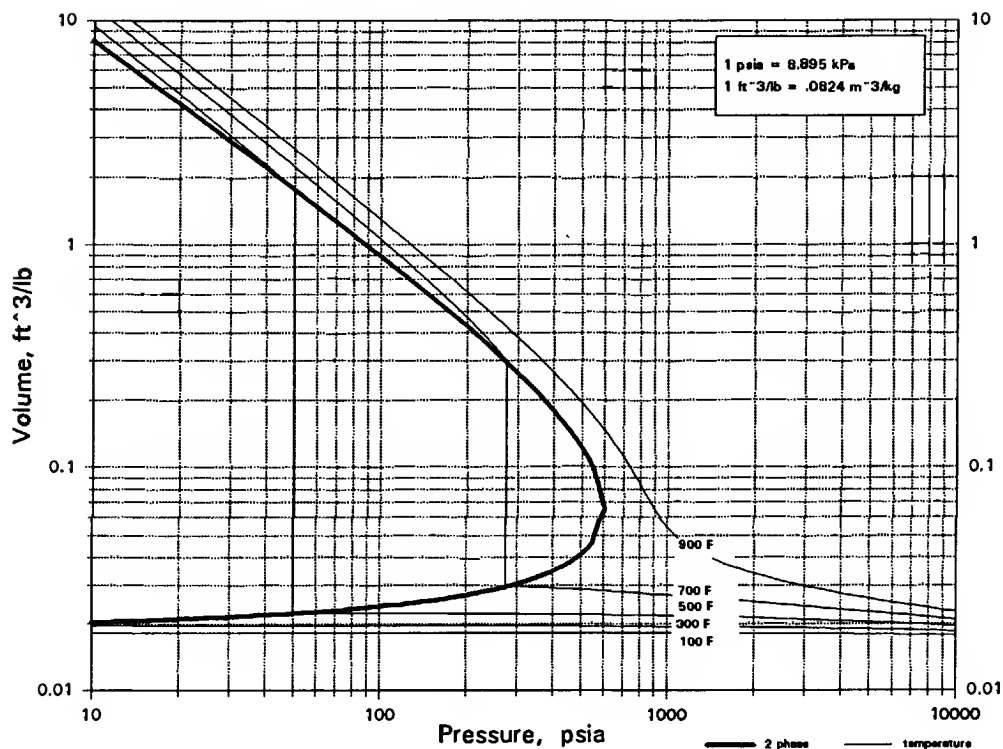
C7H9N

N-METHYLANILINE



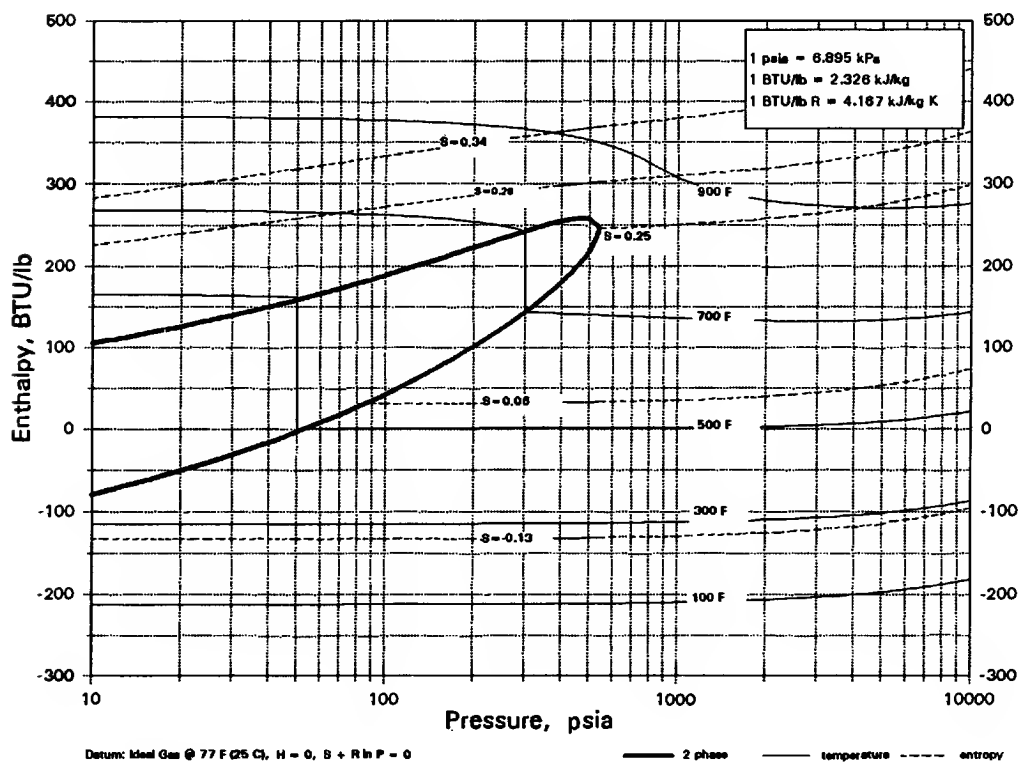
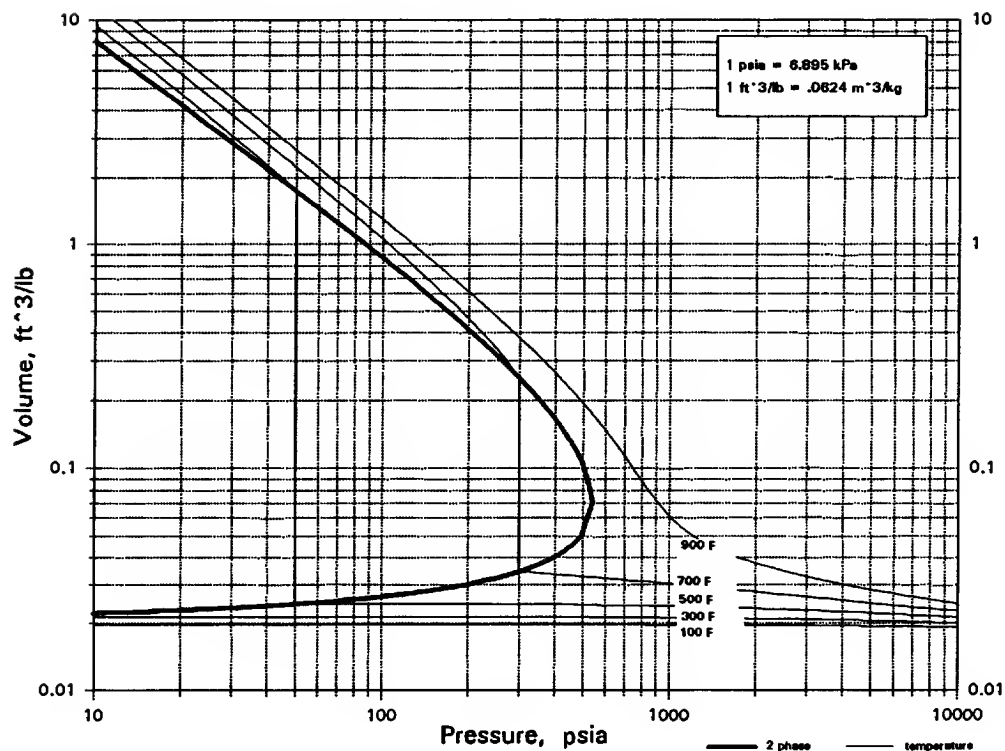
C7H9N

m-TOLUIDINE



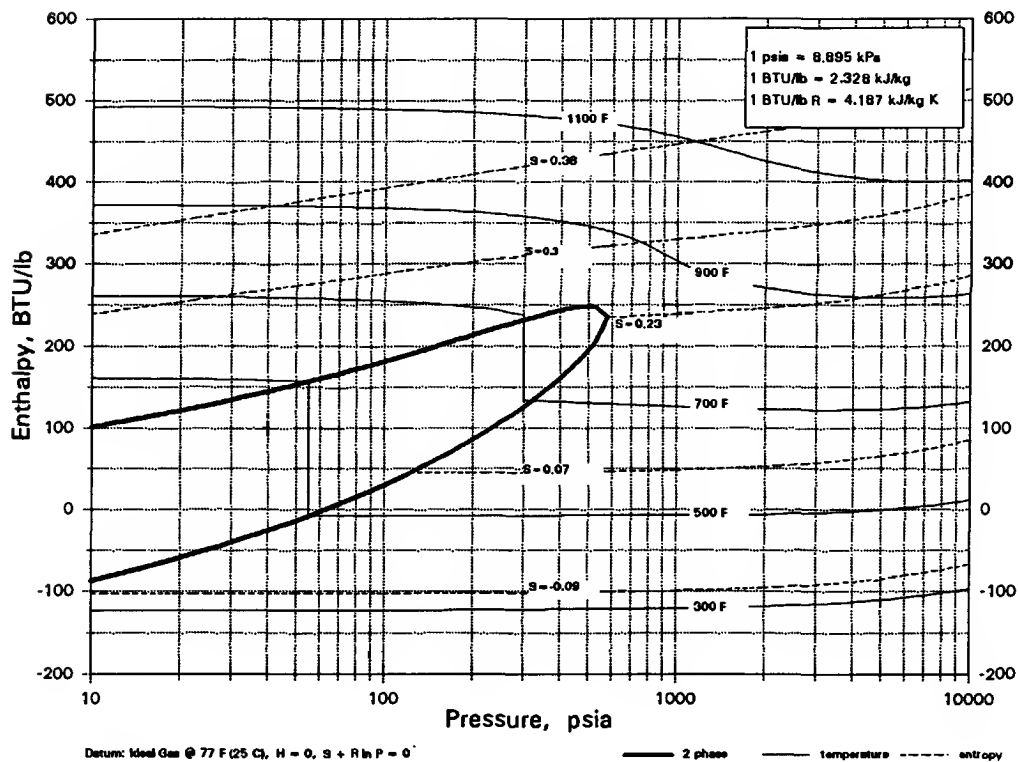
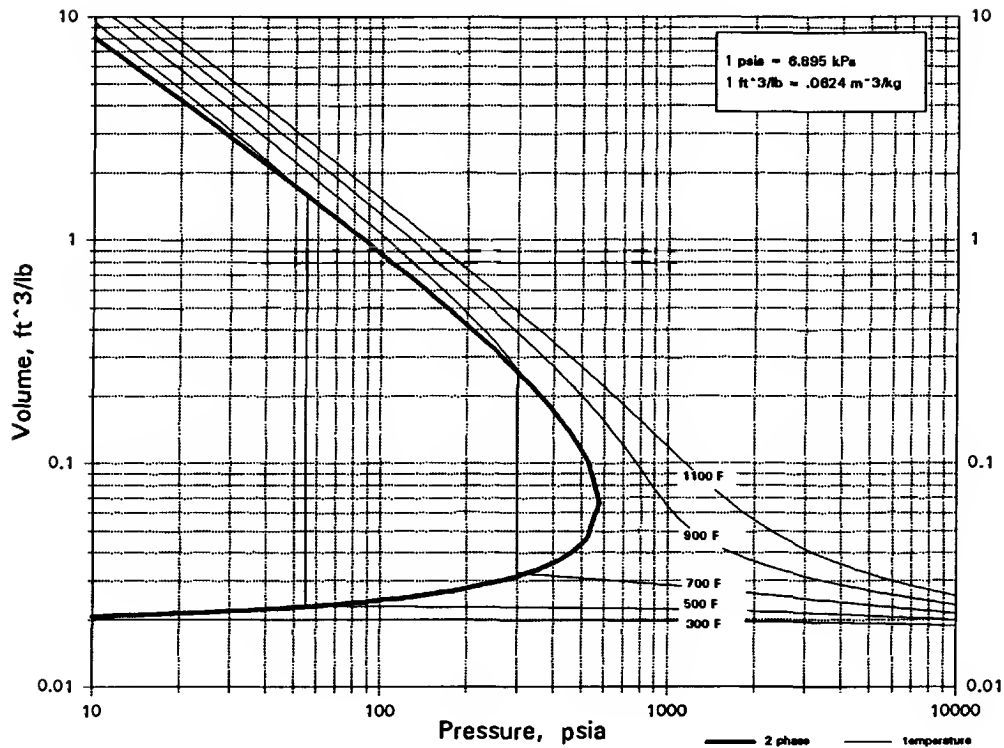
C7H9N

o-TOLUIDINE



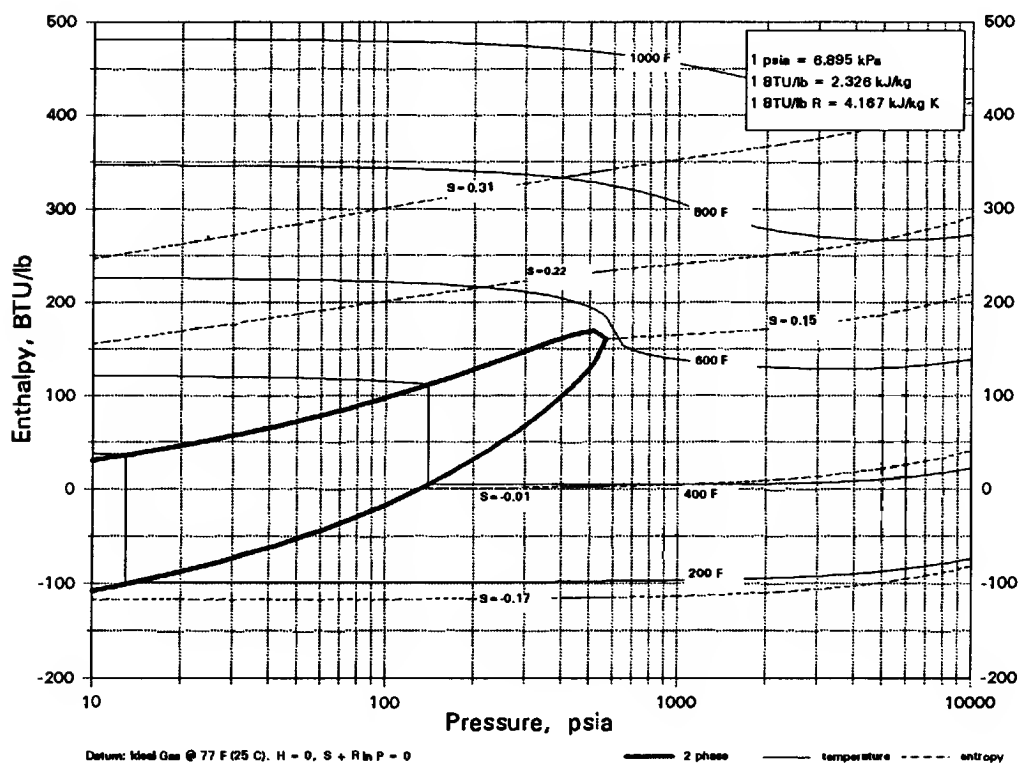
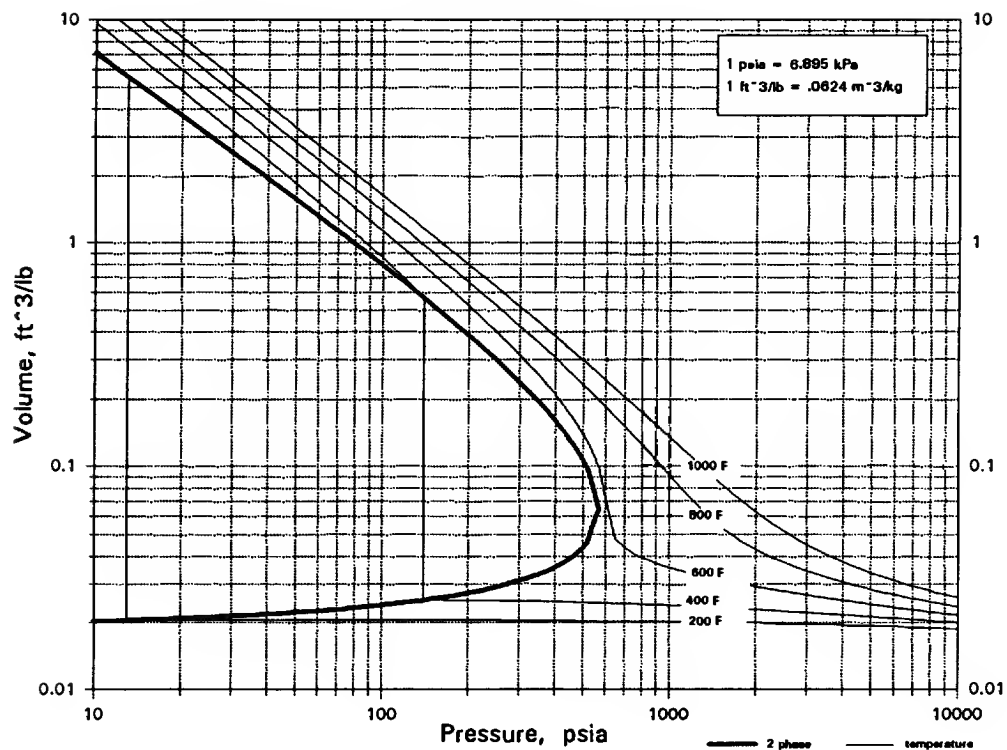
C7H9N

p-TOLUIDINE



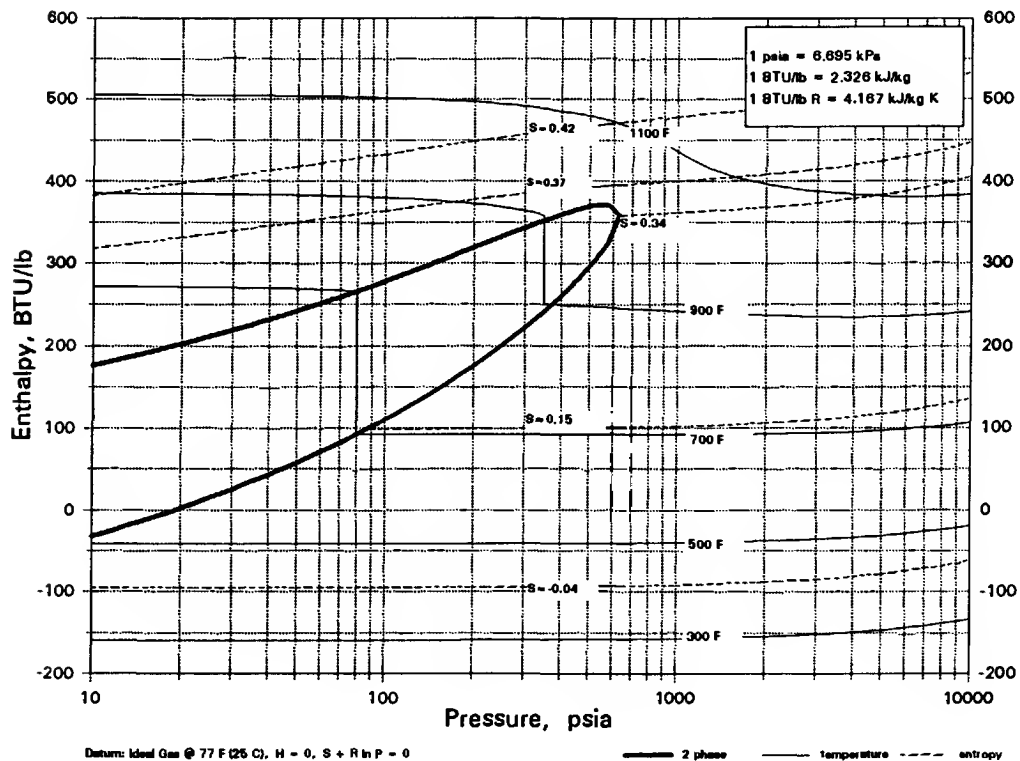
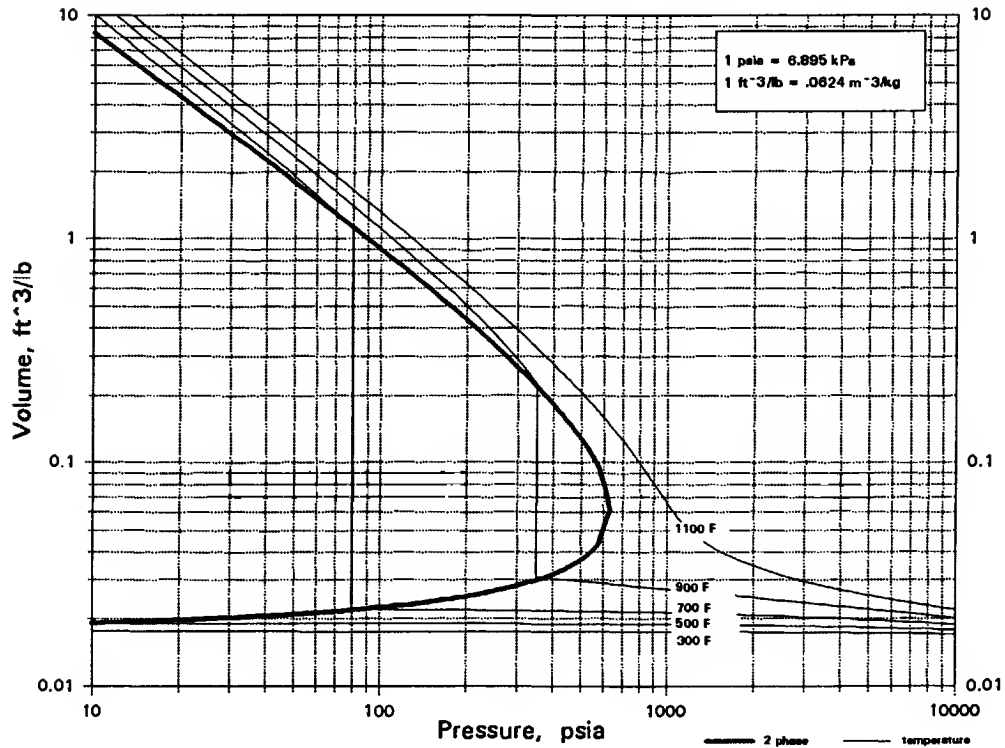
C7H10

2-NORBORNENE



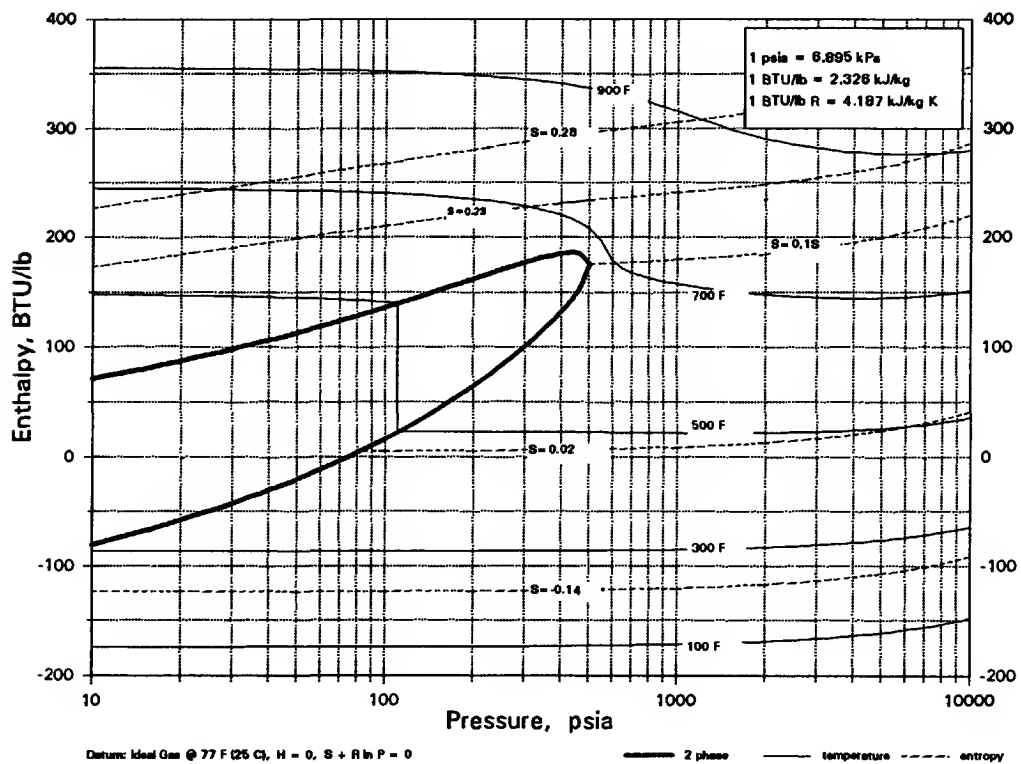
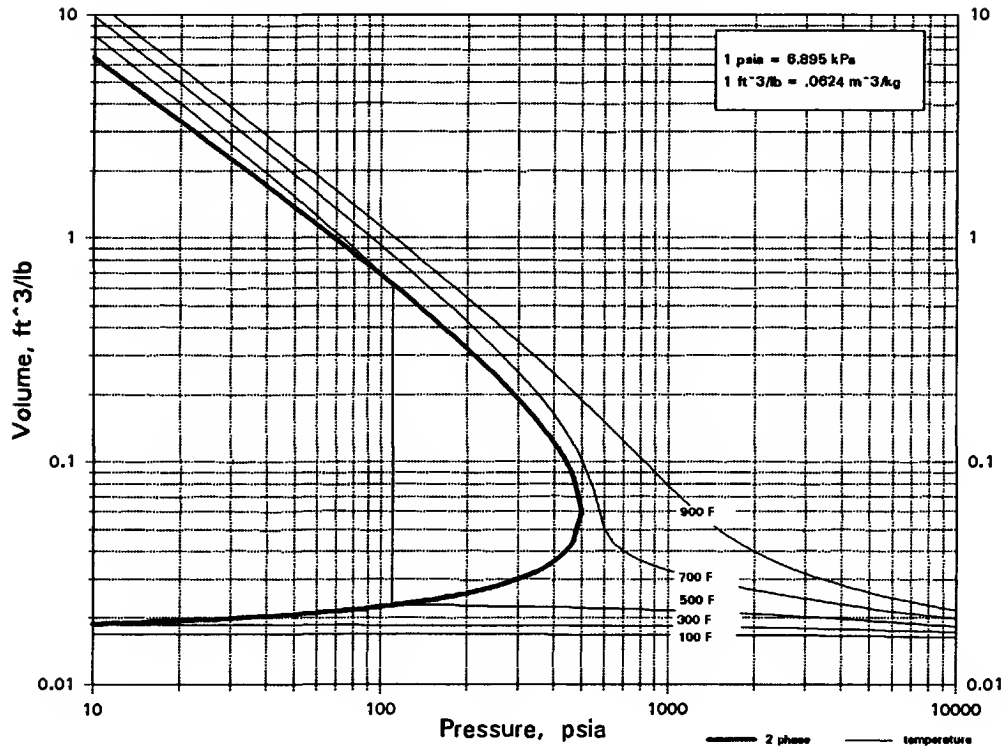
C7H10N2

TOLUENEDIAMINE



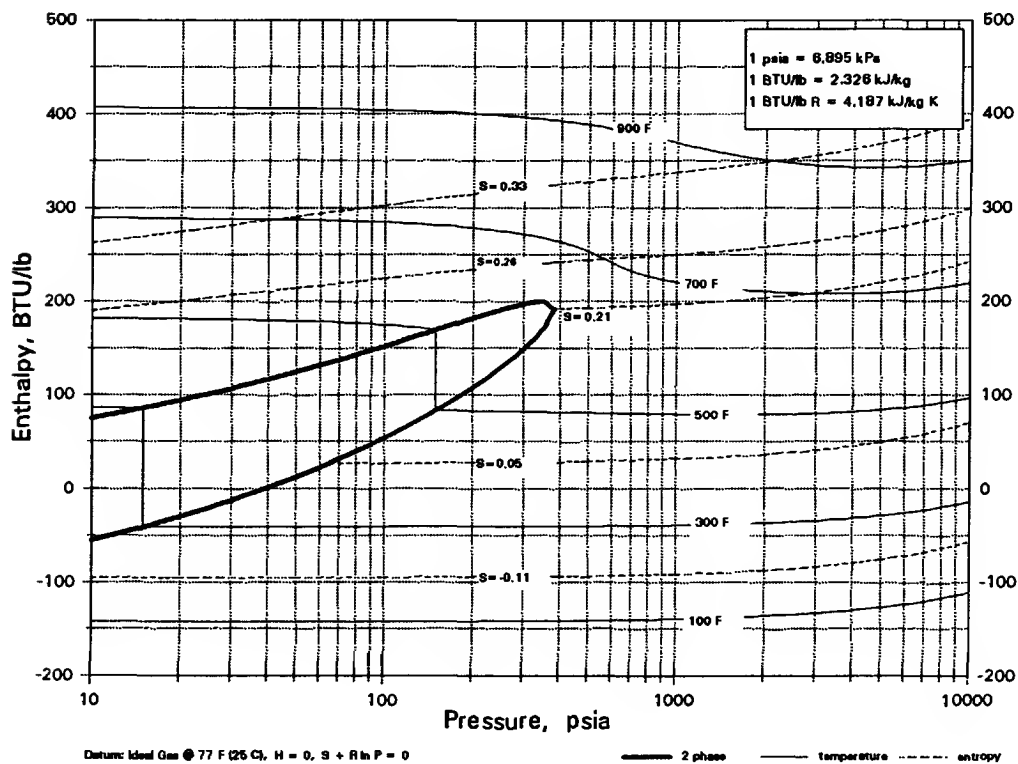
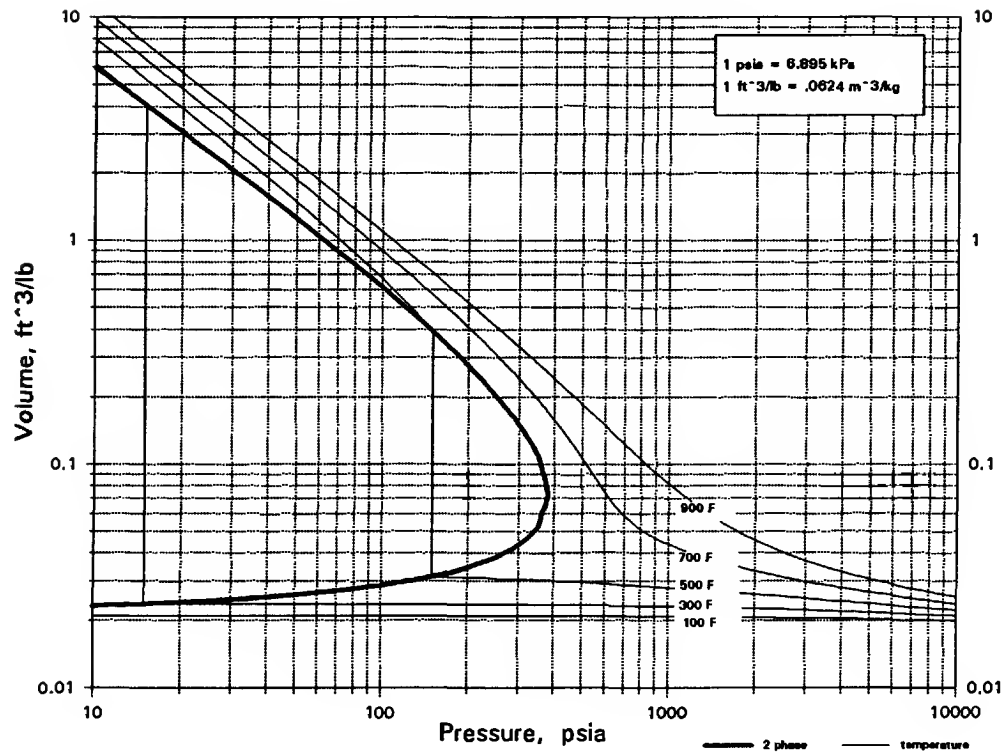
C7H11NO

CYCLOHEXYL ISOCYANATE



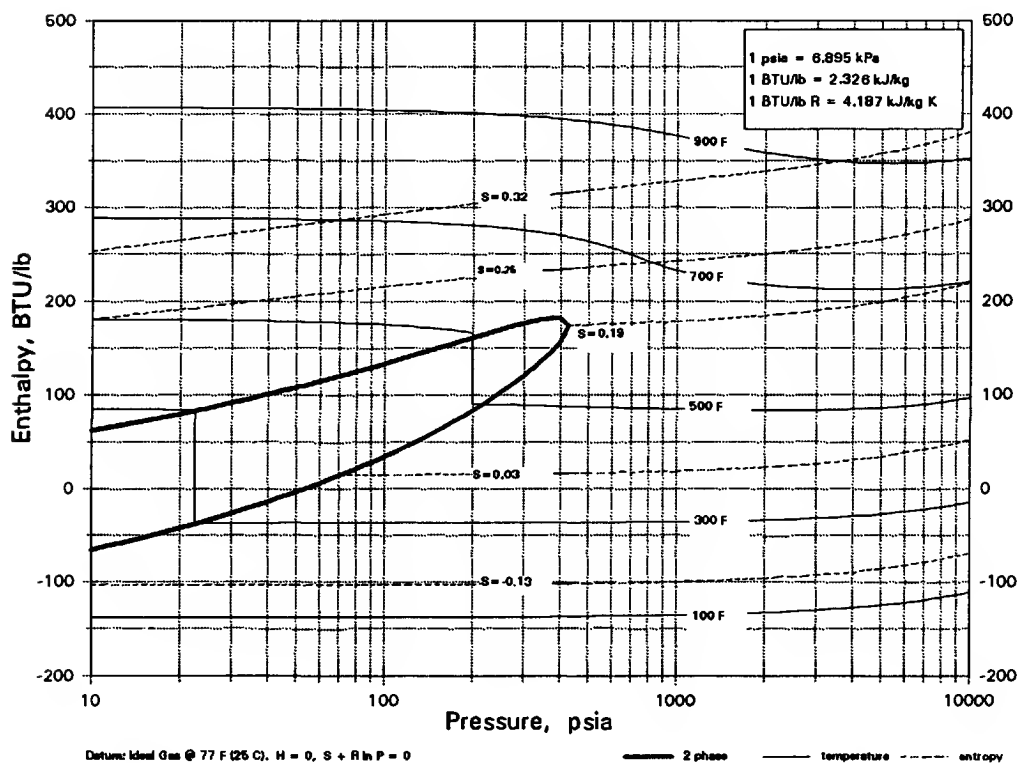
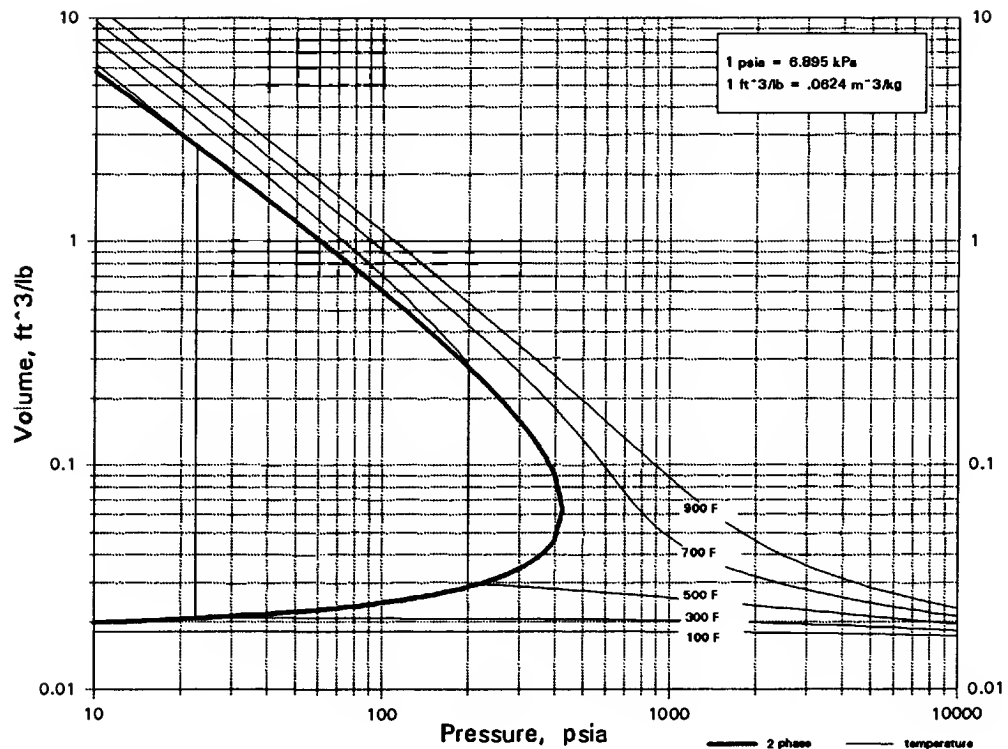
C7H12O2

n-BUTYL ACRYLATE



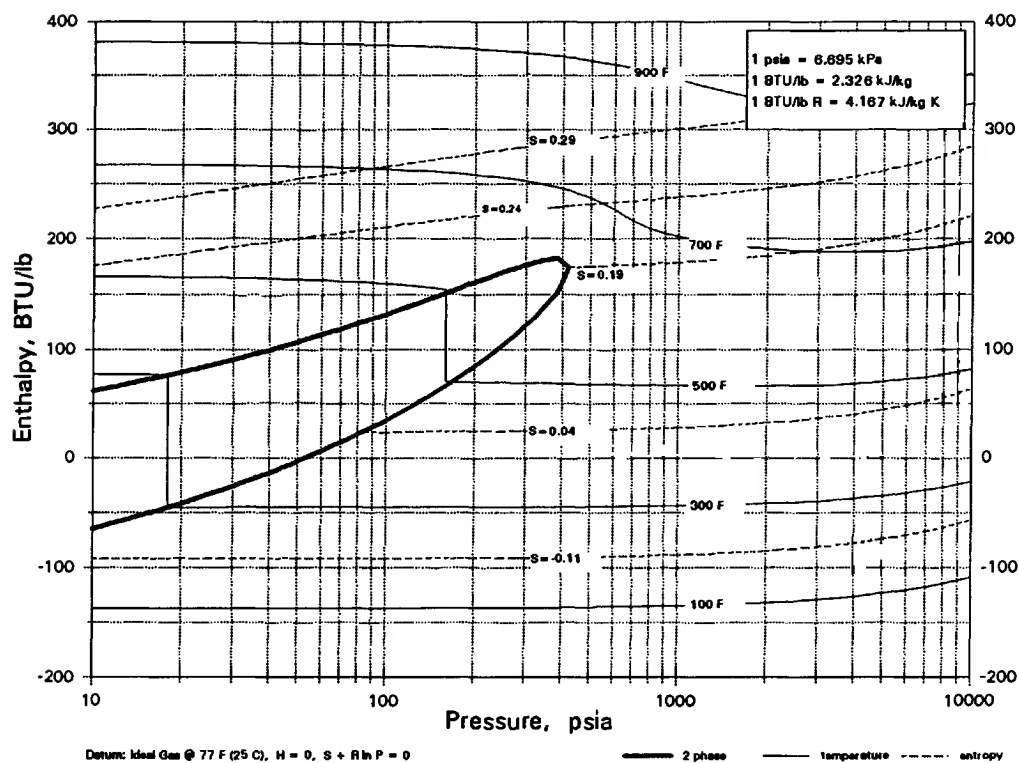
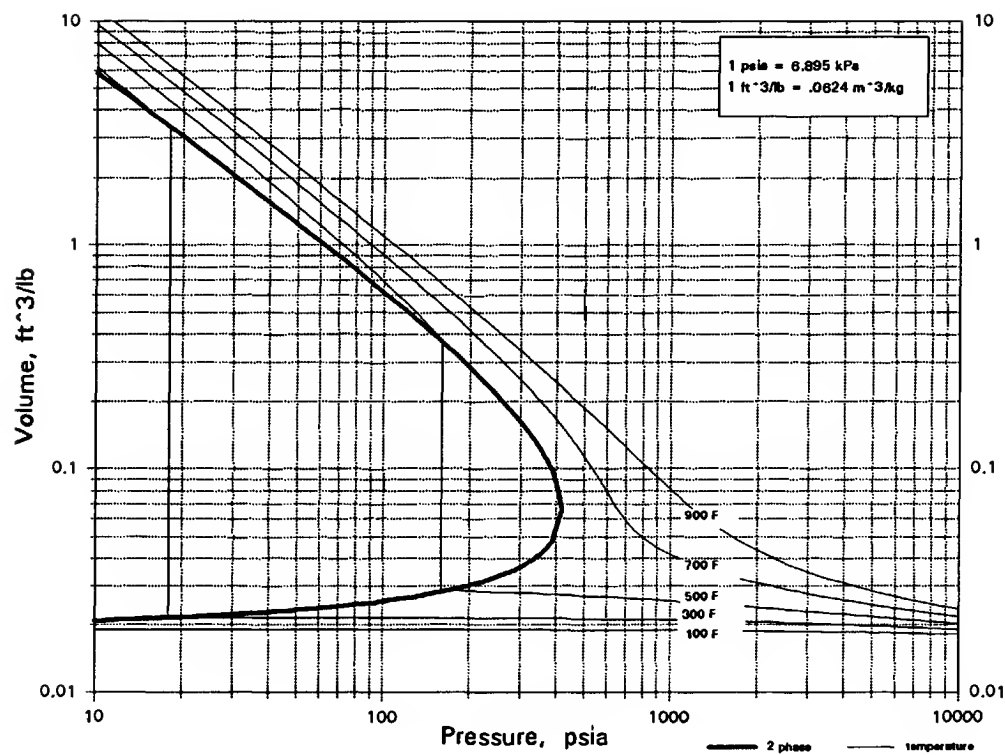
C7H12O2

ISOBUTYL ACRYLATE



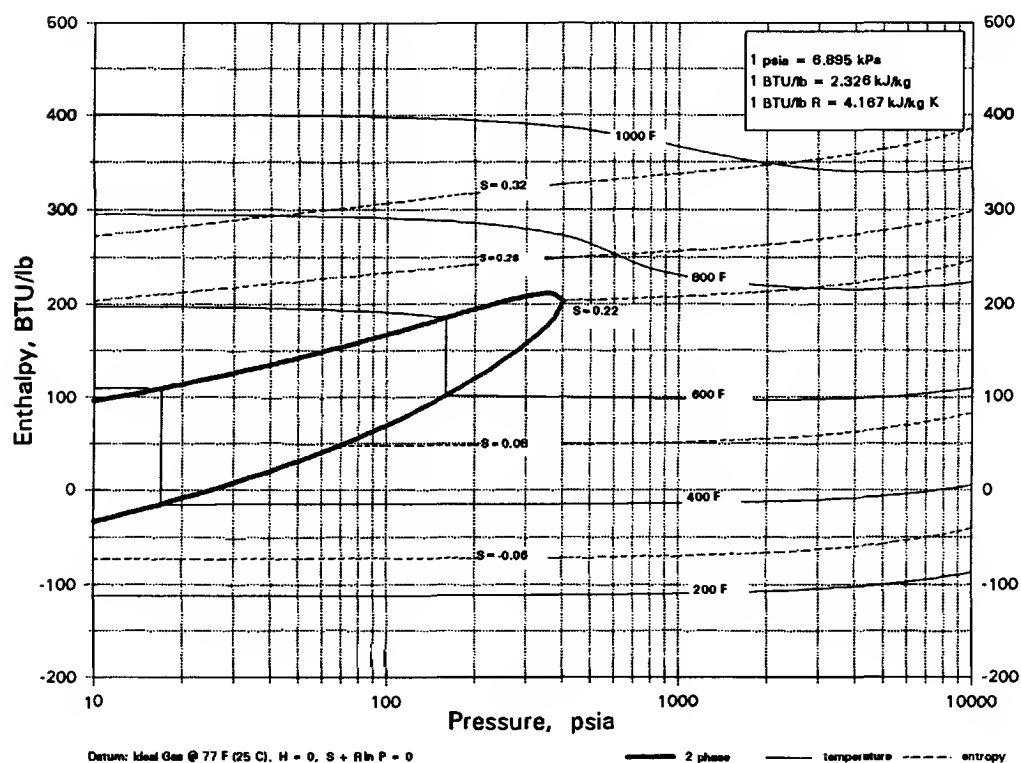
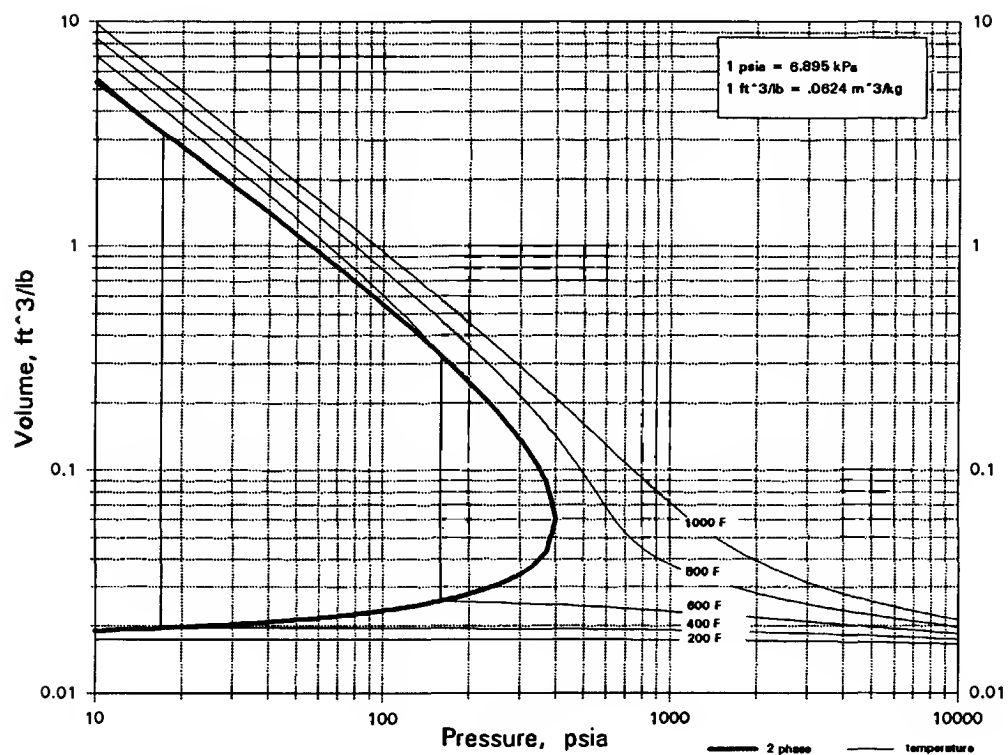
C7H12O2

n-PROPYL METHACRYLATE



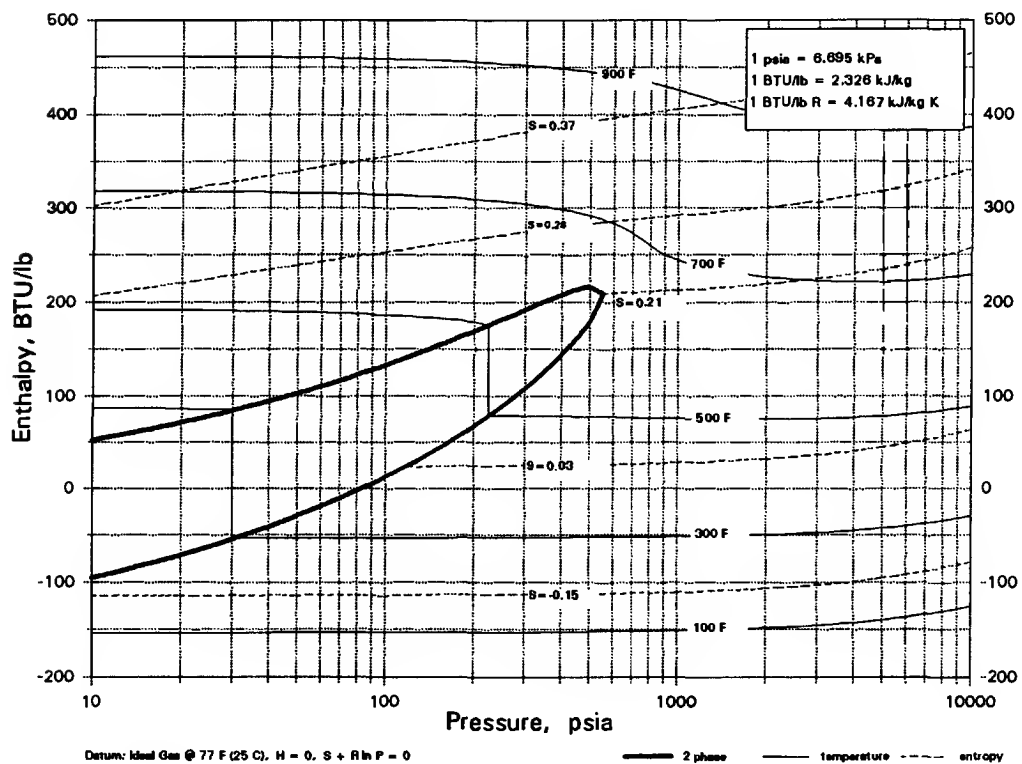
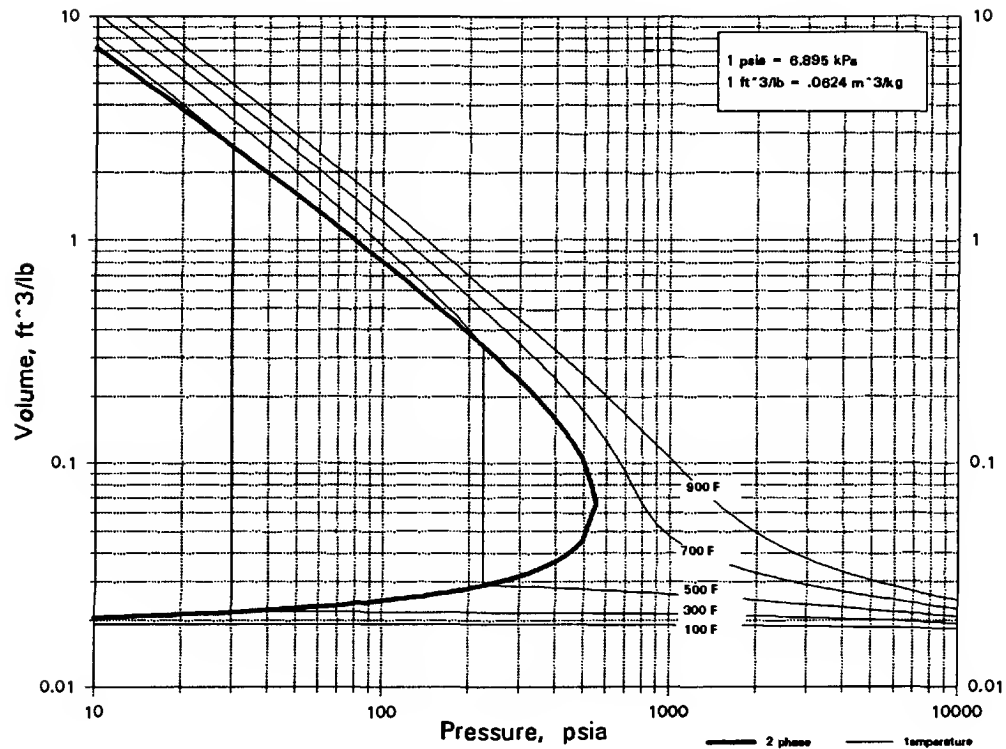
C7H12O4

DIETHYL MALONATE



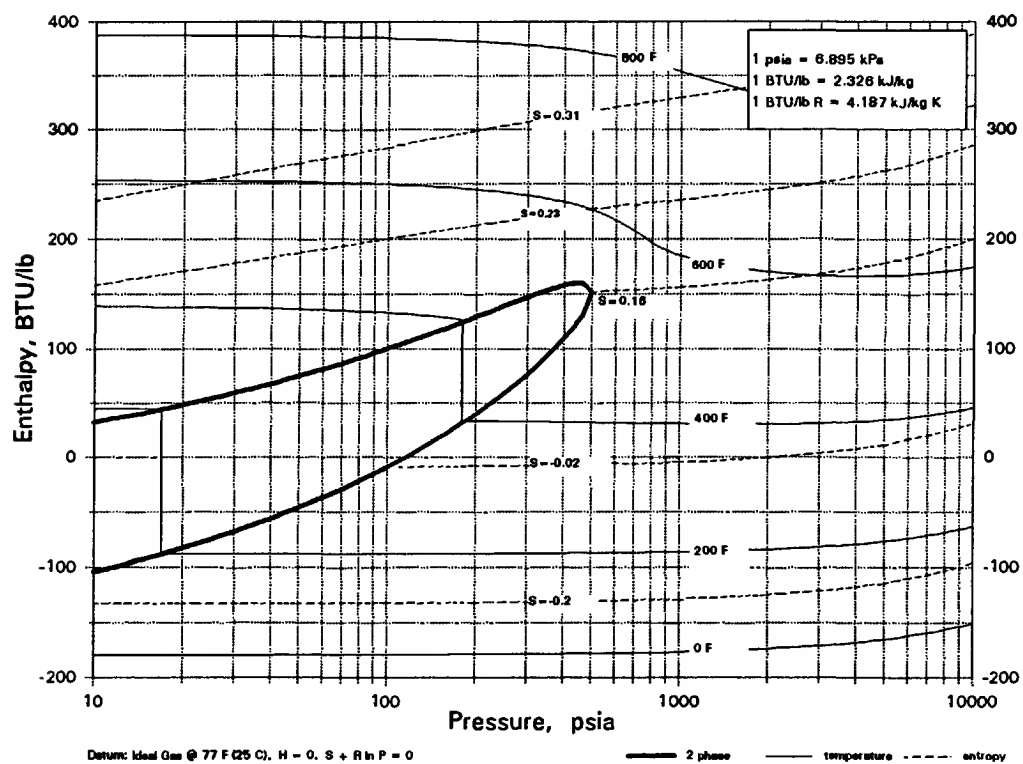
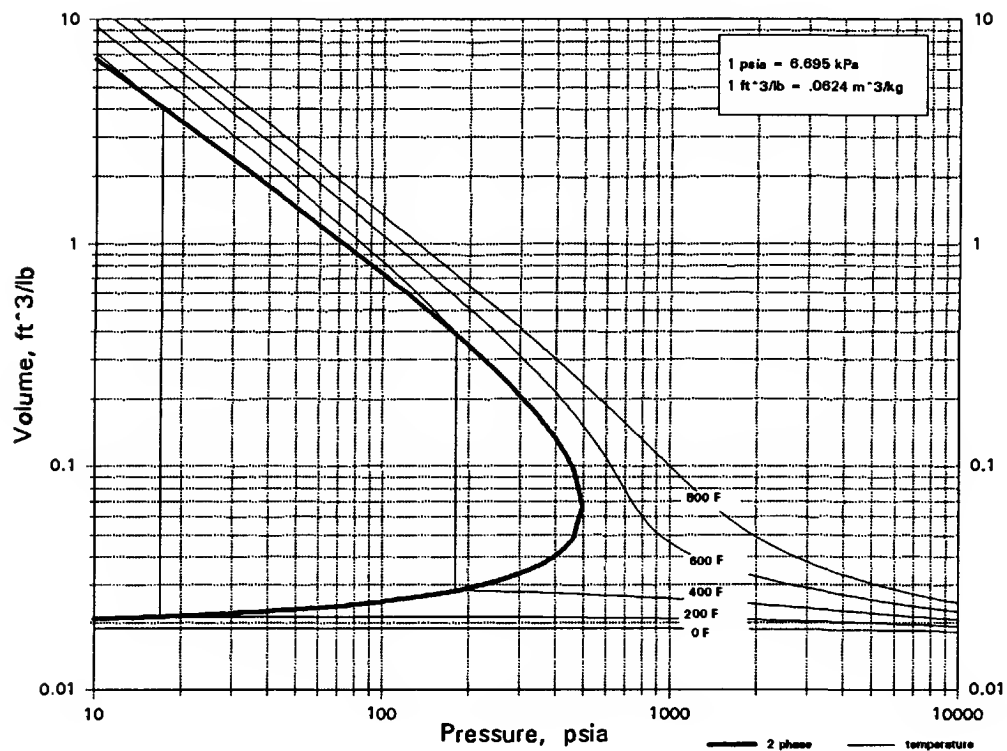
C7H14

CYCLOHEPTANE



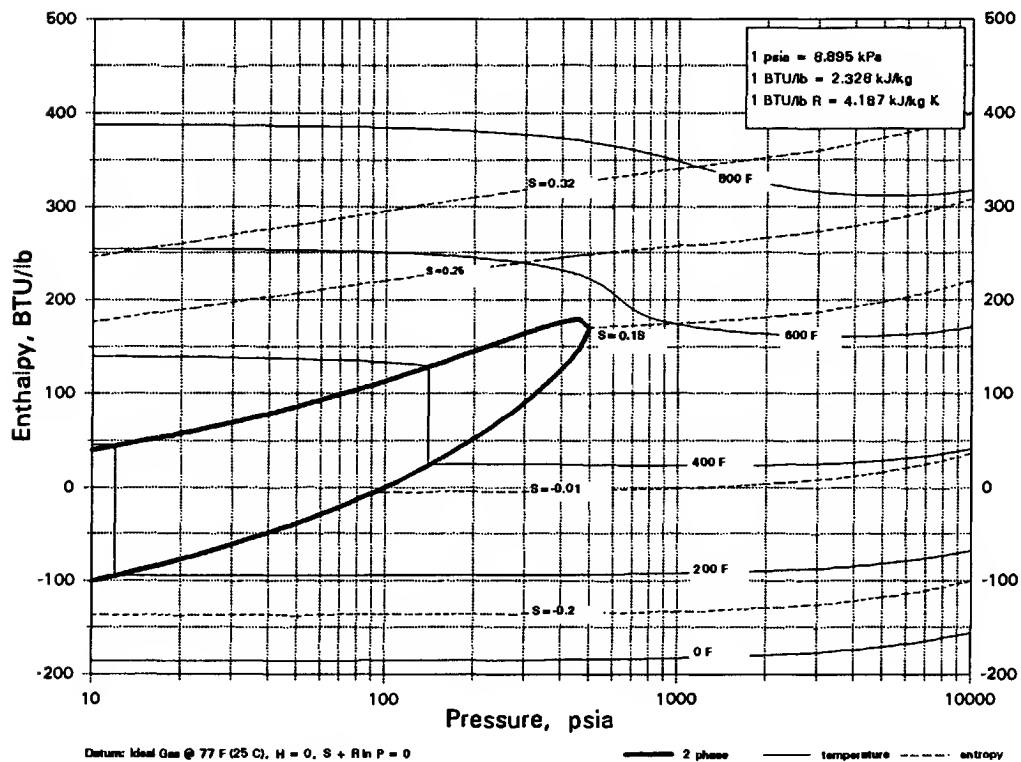
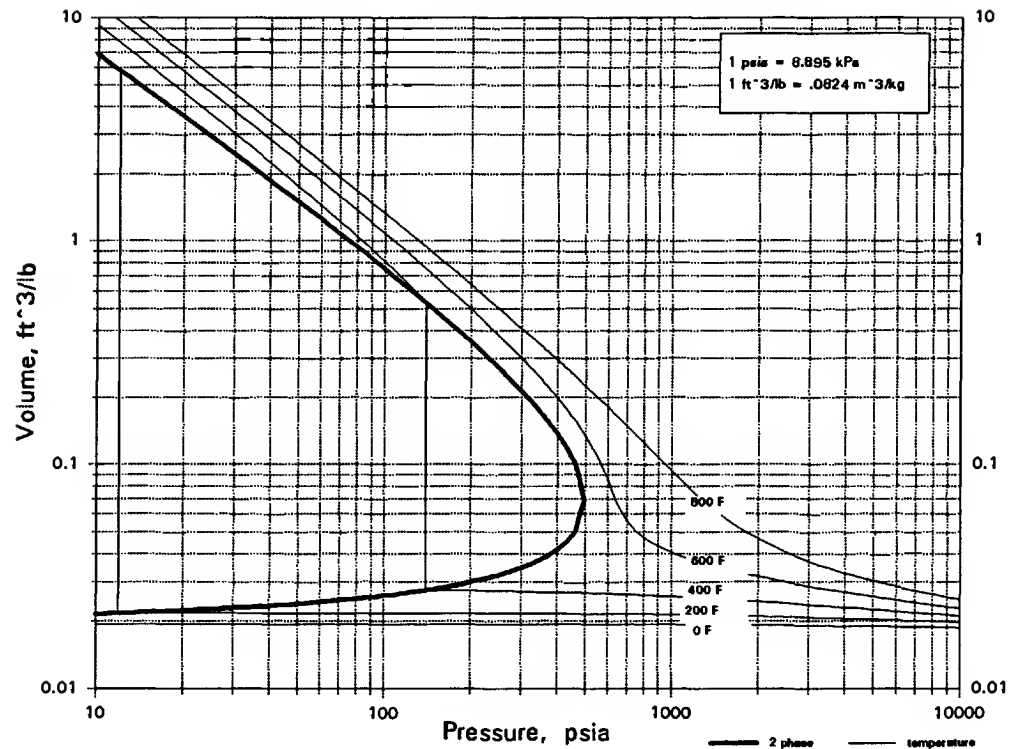
C7H14

1-1-DIMETHYLCYCLOPENTANE



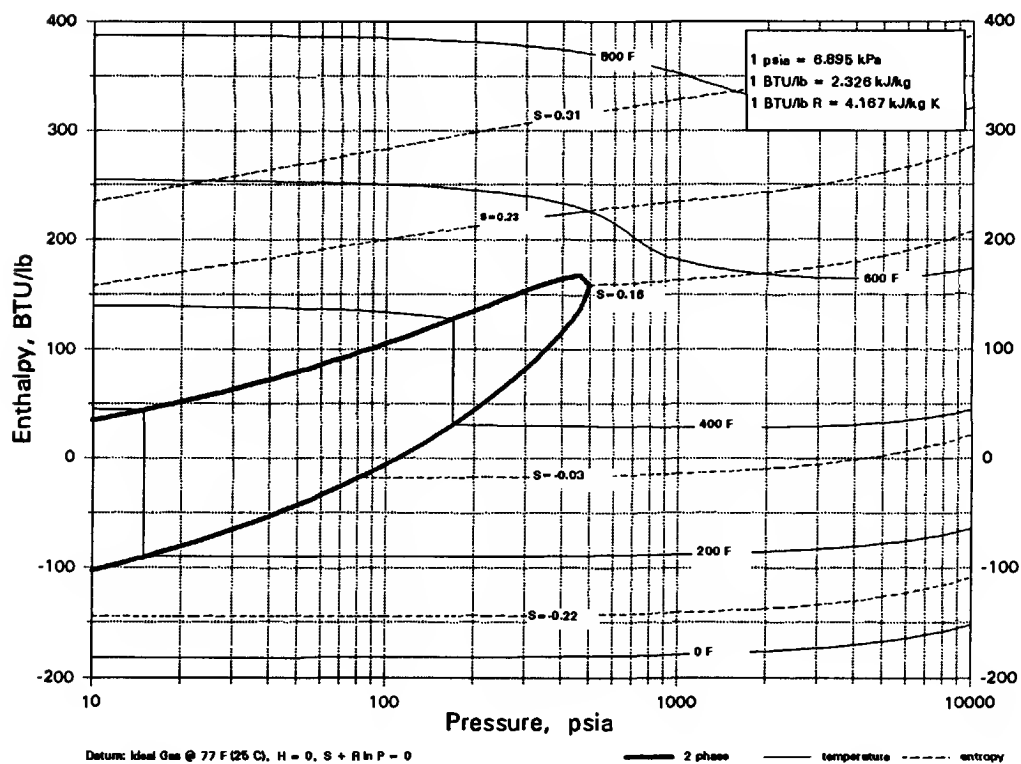
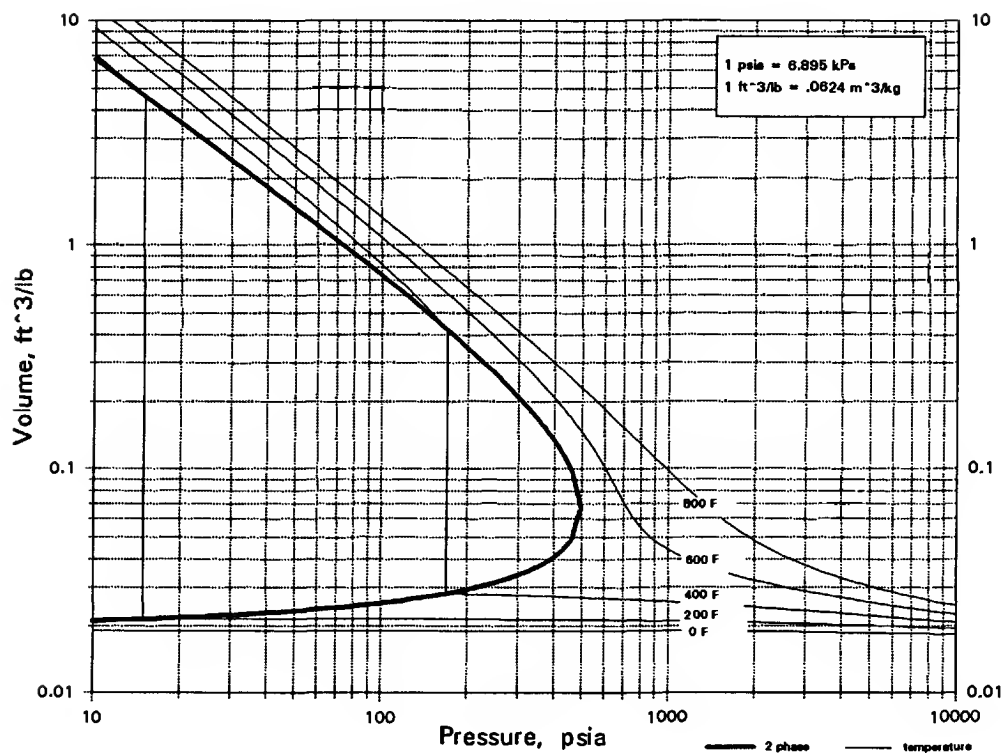
C7H14

cis-1-2-DIMETHYLCYCLOPENTANE



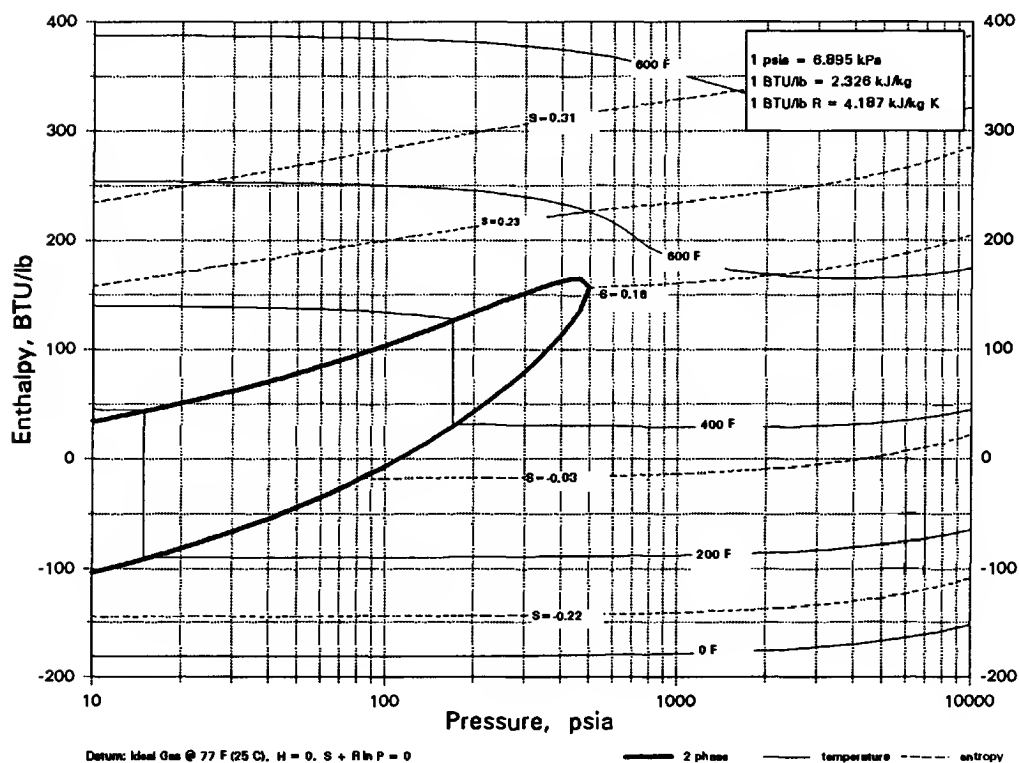
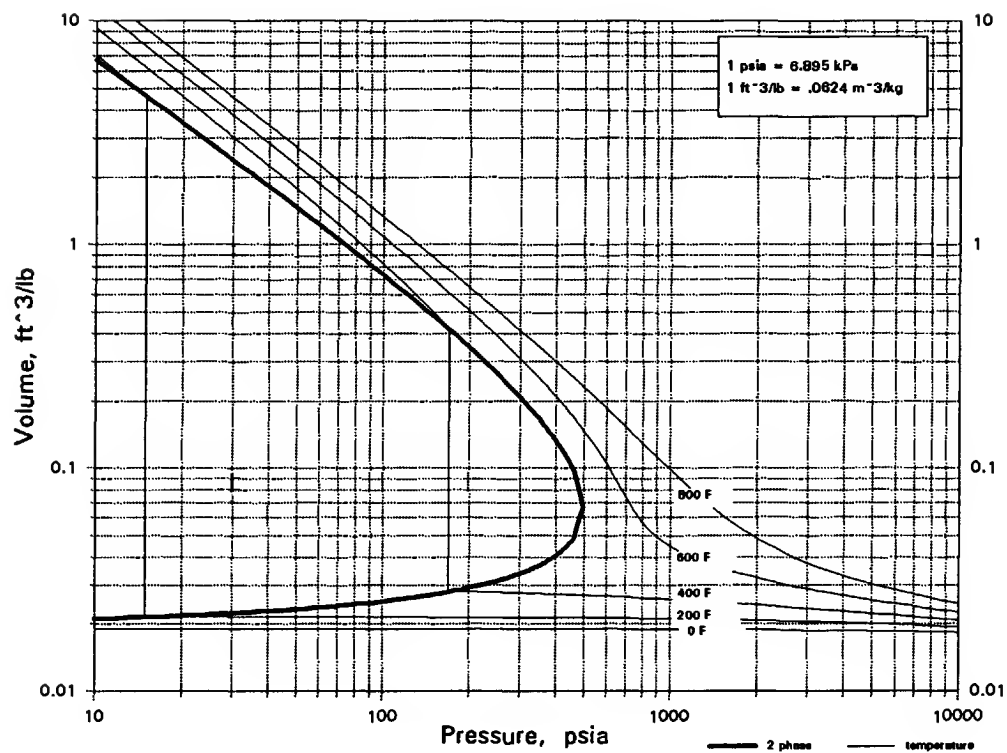
C7H14

trans-1-2-DIMETHYLCYCLOPENTANE



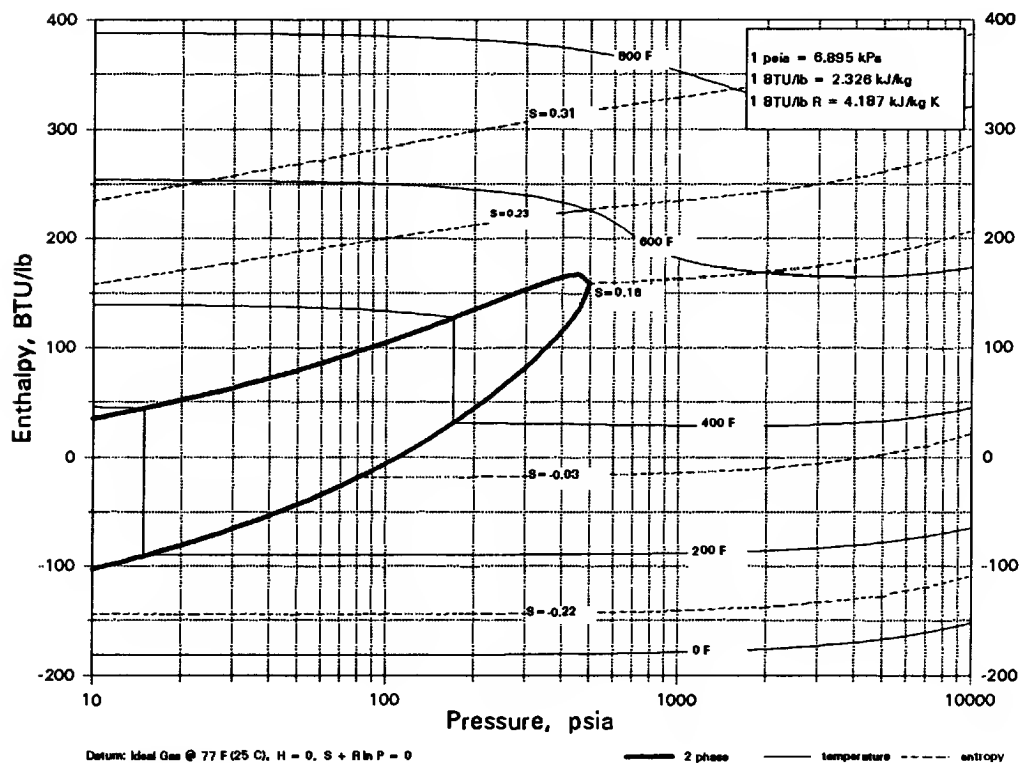
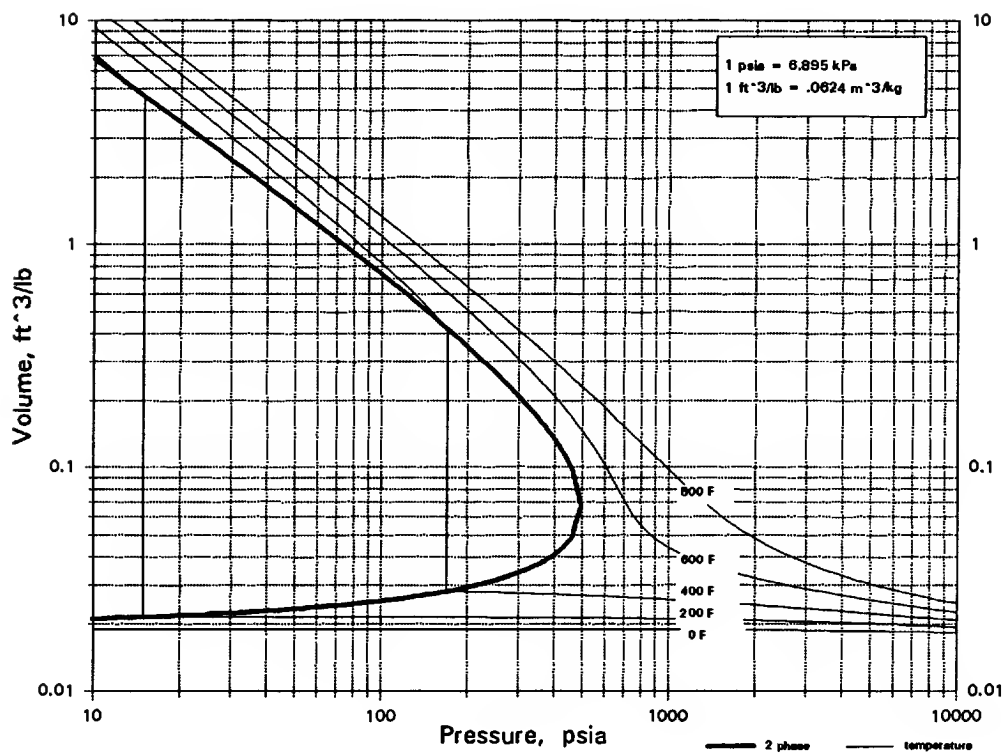
C7H14

cis-1-3-DIMETHYLCYCLOPENTANE



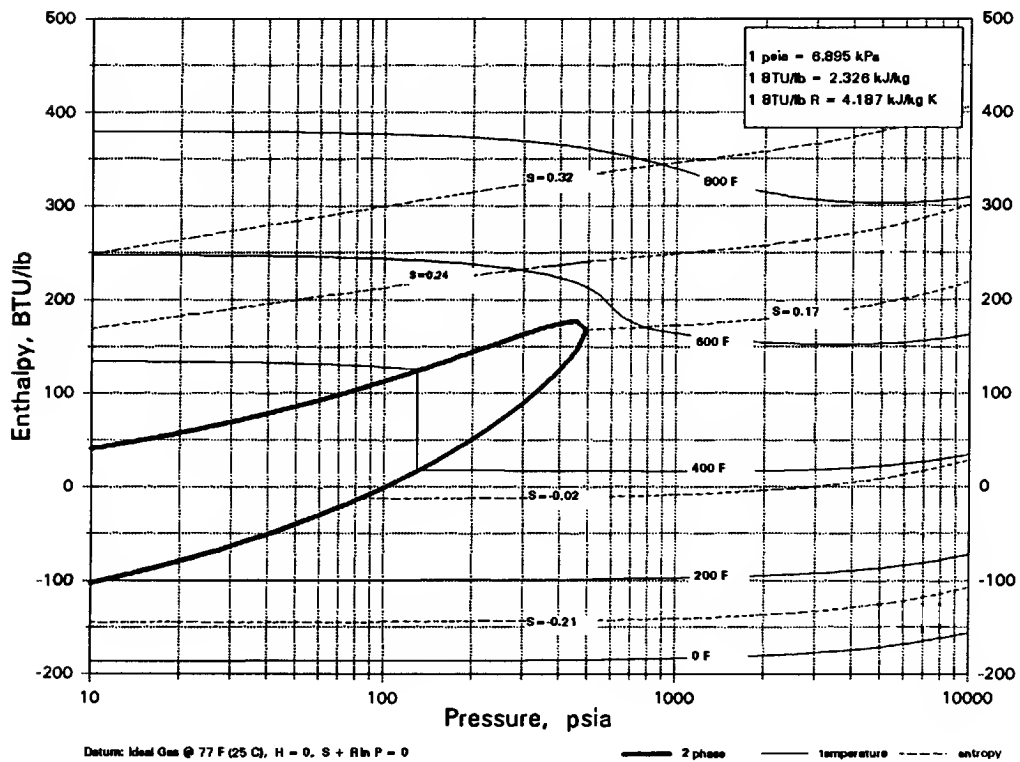
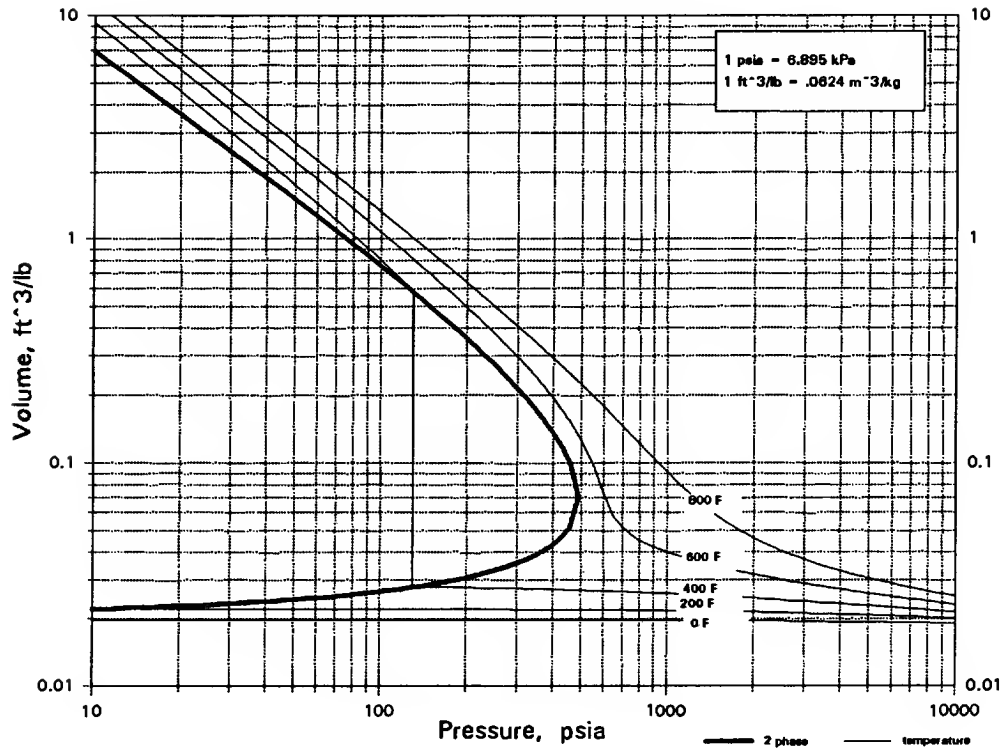
C7H14

trans-1-3-DIMETHYLCYCLOPENTANE



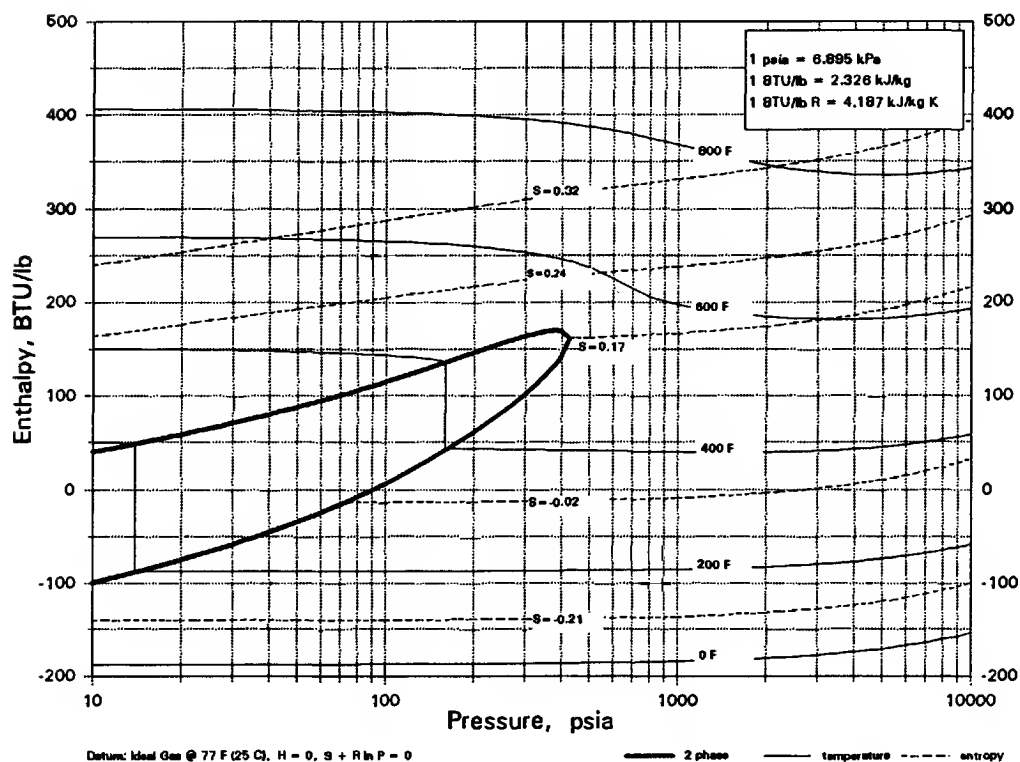
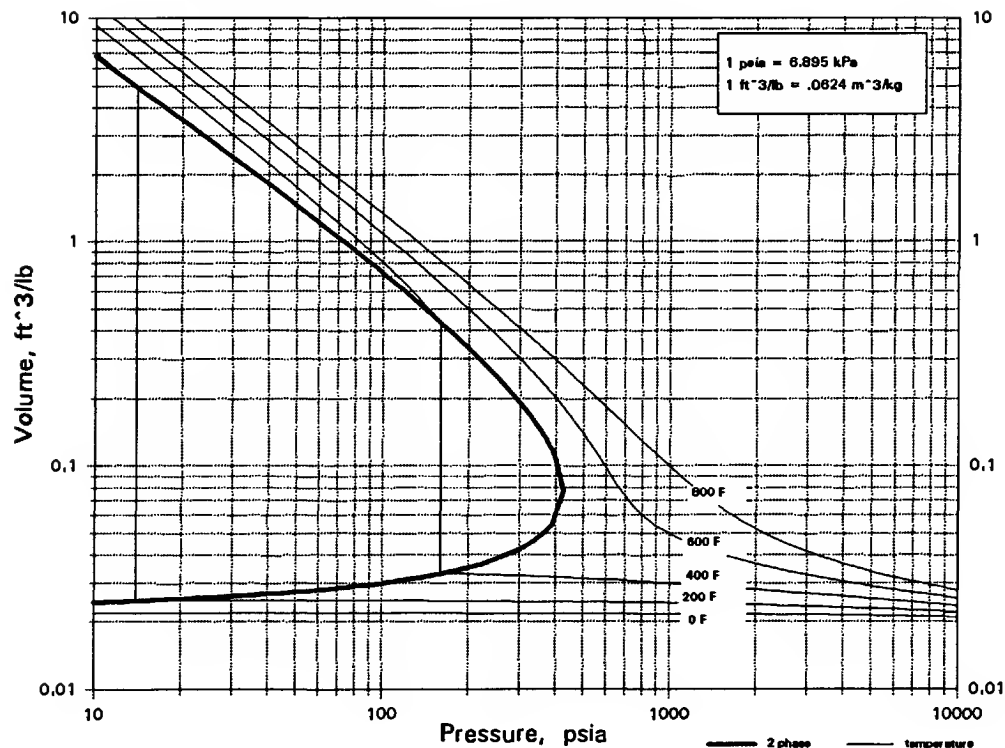
C7H14

ETHYLCYCLOPENTANE



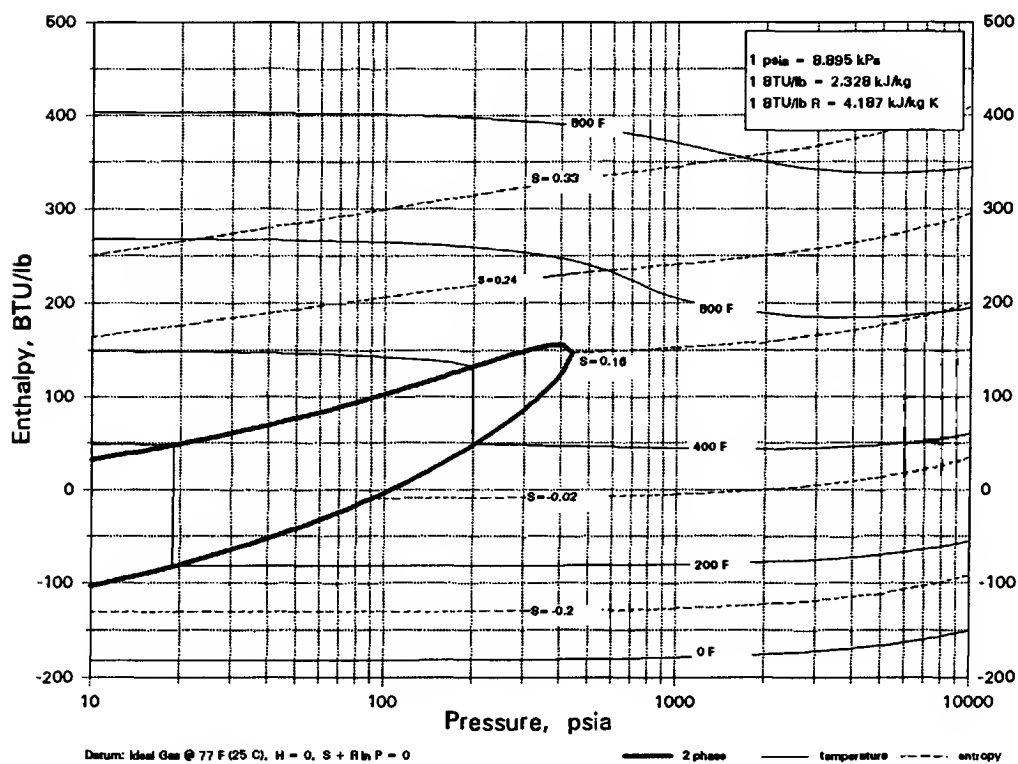
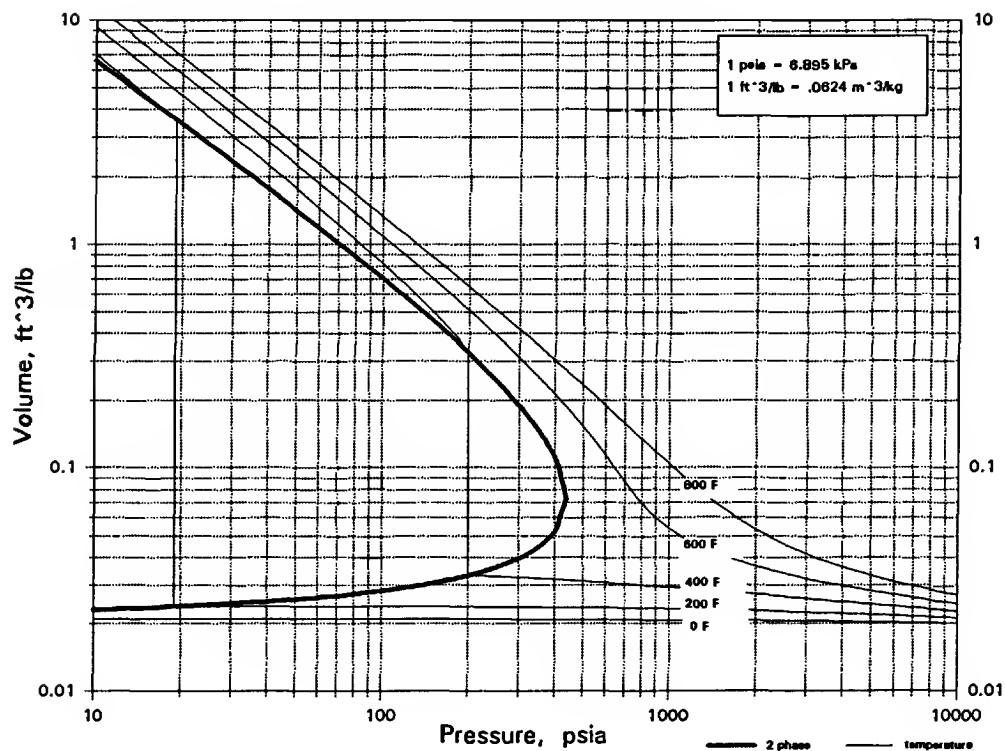
C7H14

2-ETHYL-1-PENTENE



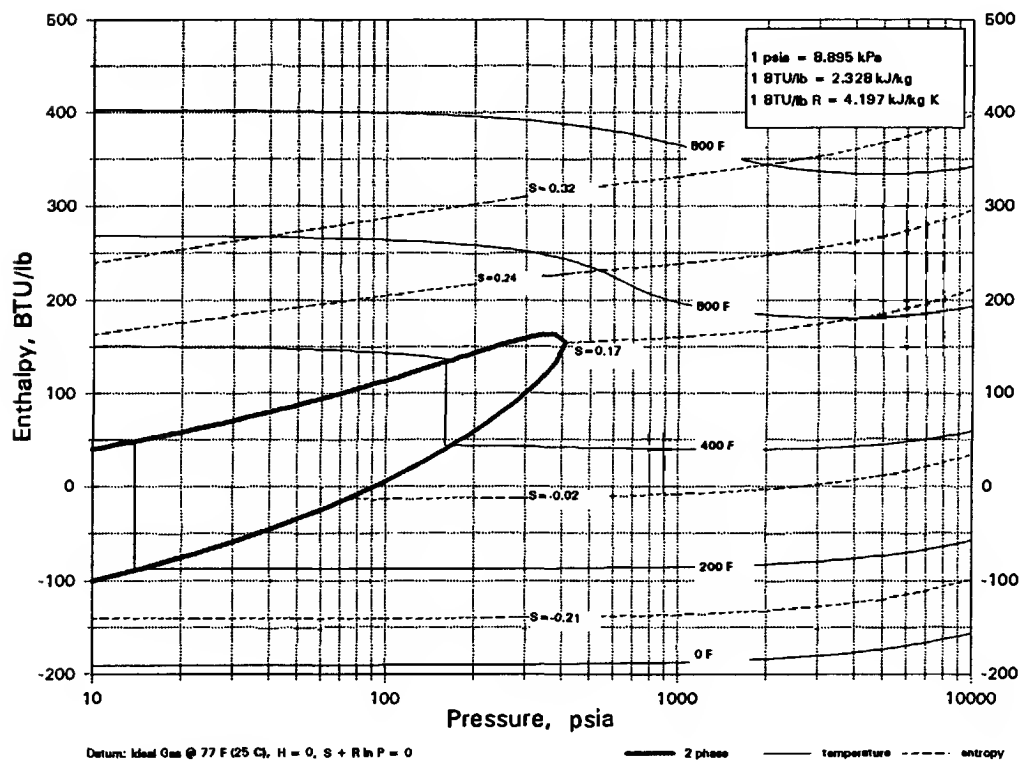
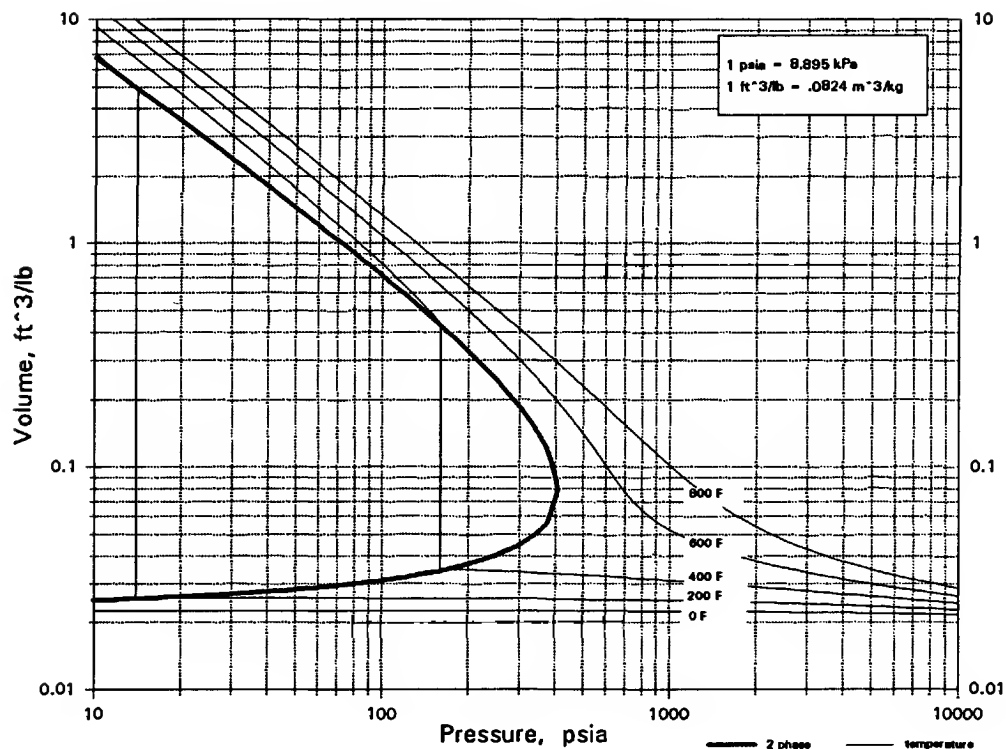
C7H14

3-ETHYL-1-PENTENE



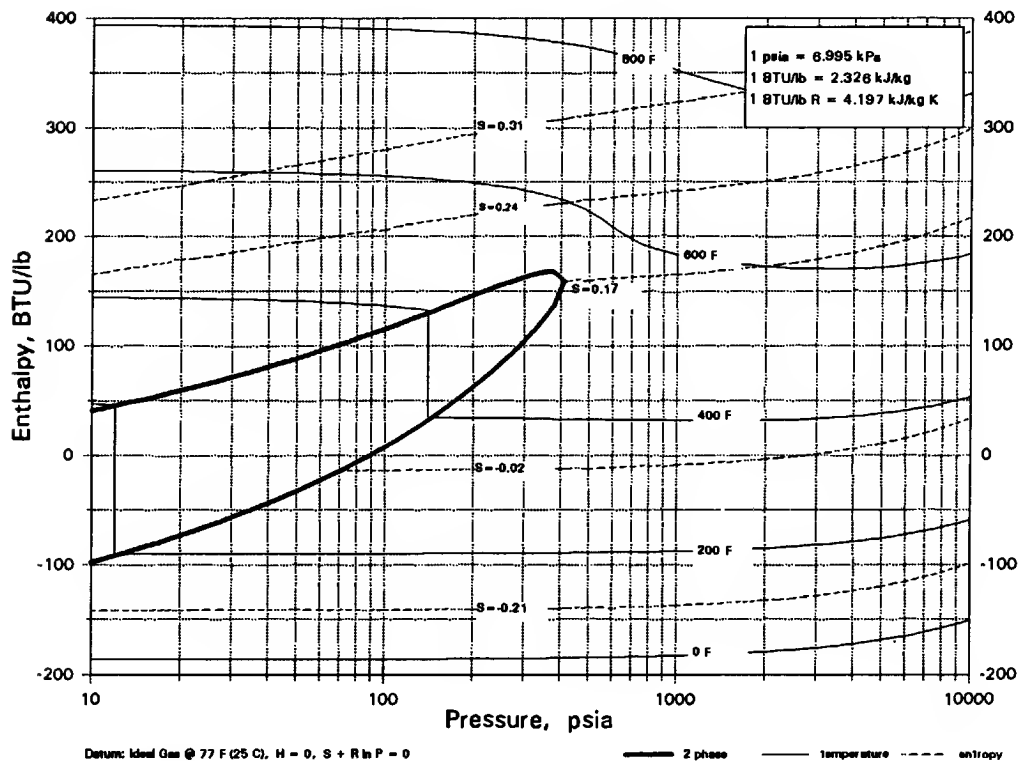
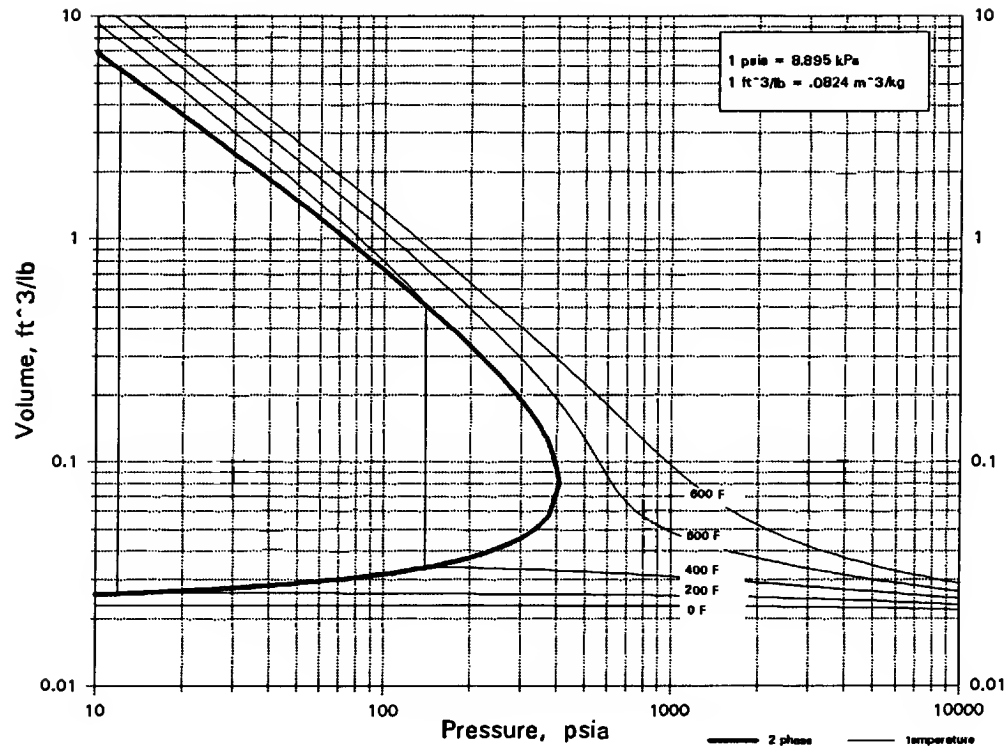
C7H14

1-HEPTENE



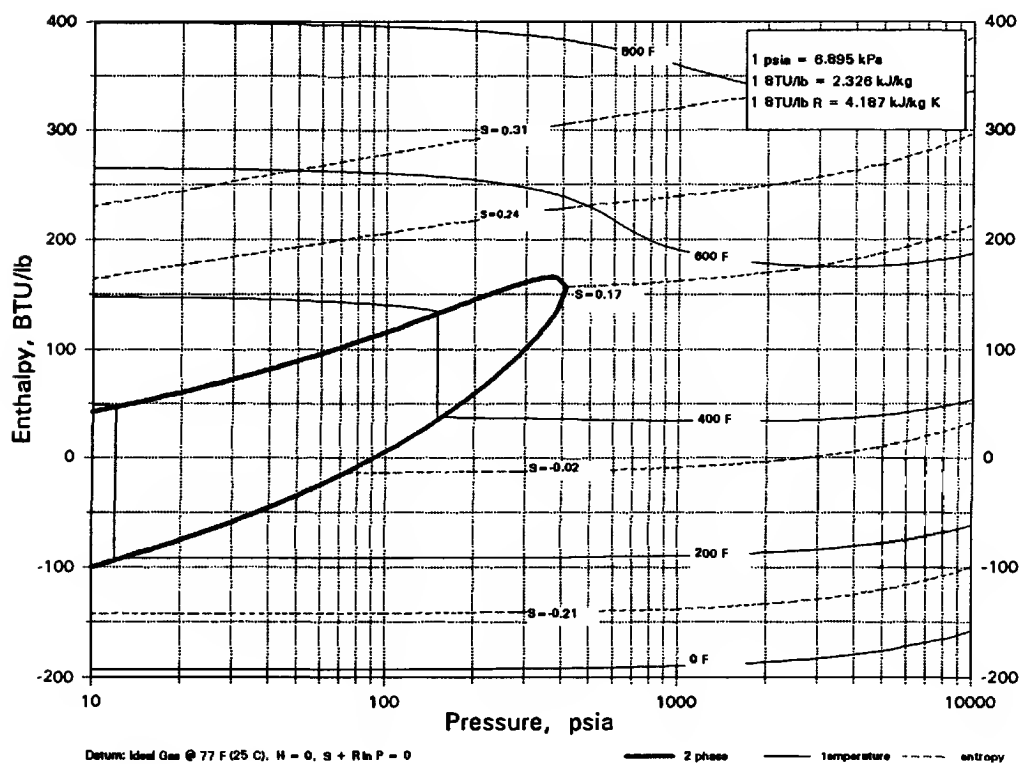
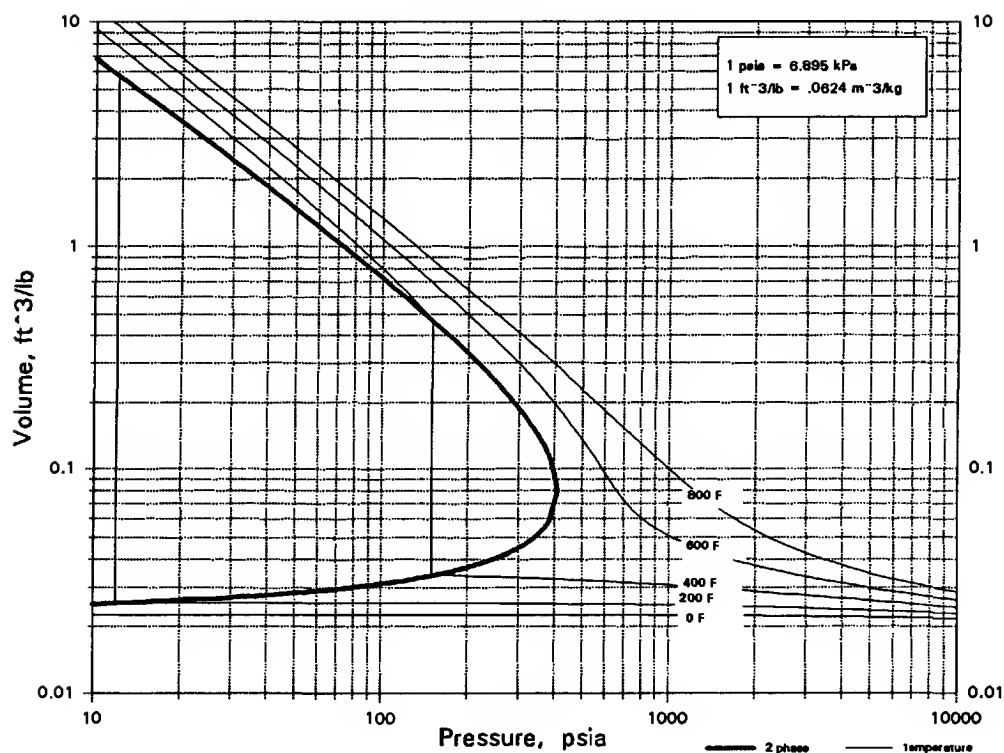
C7H14

cis-2-HEPTENE

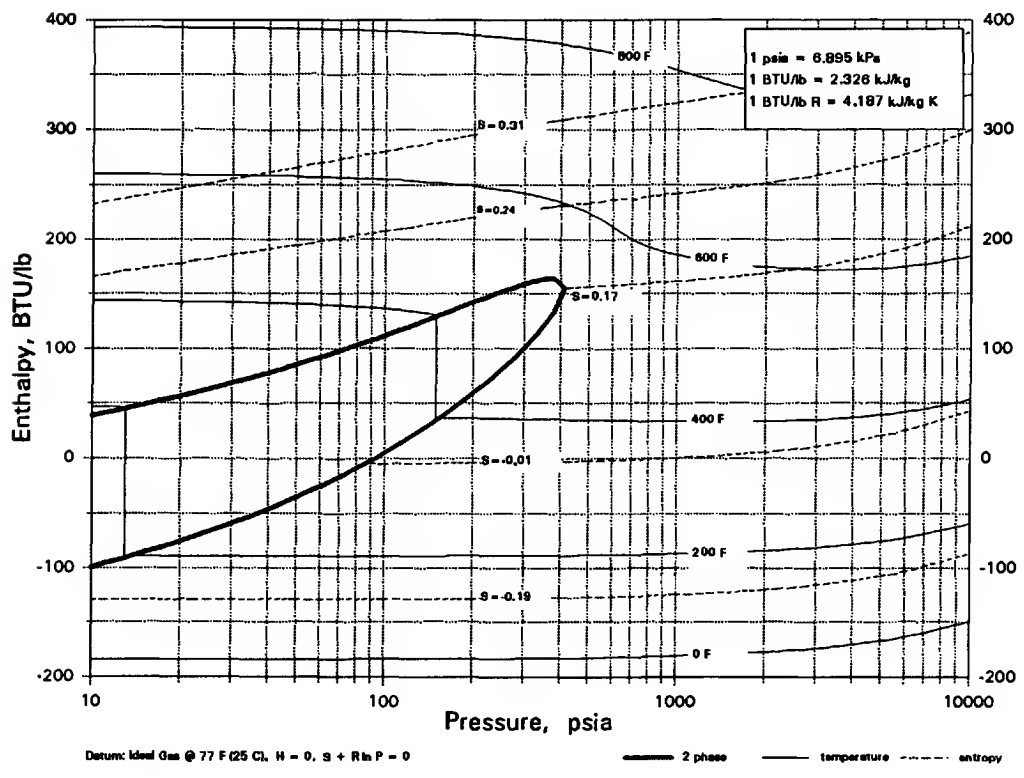
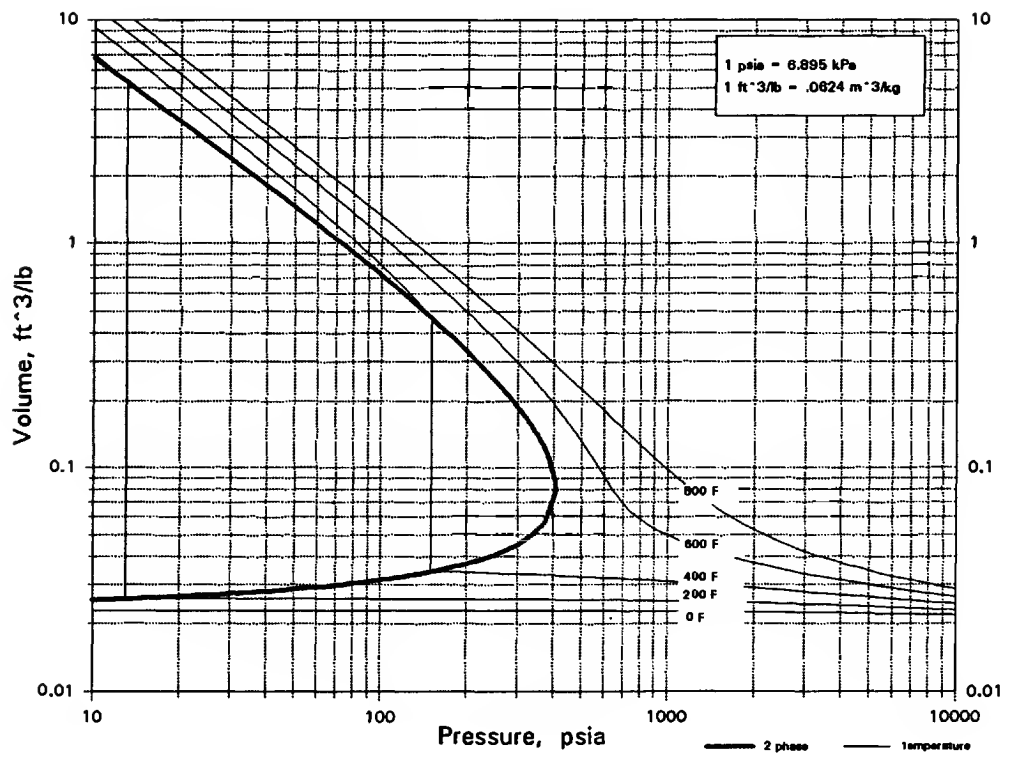


C7H14

trans-2-HEPTENE

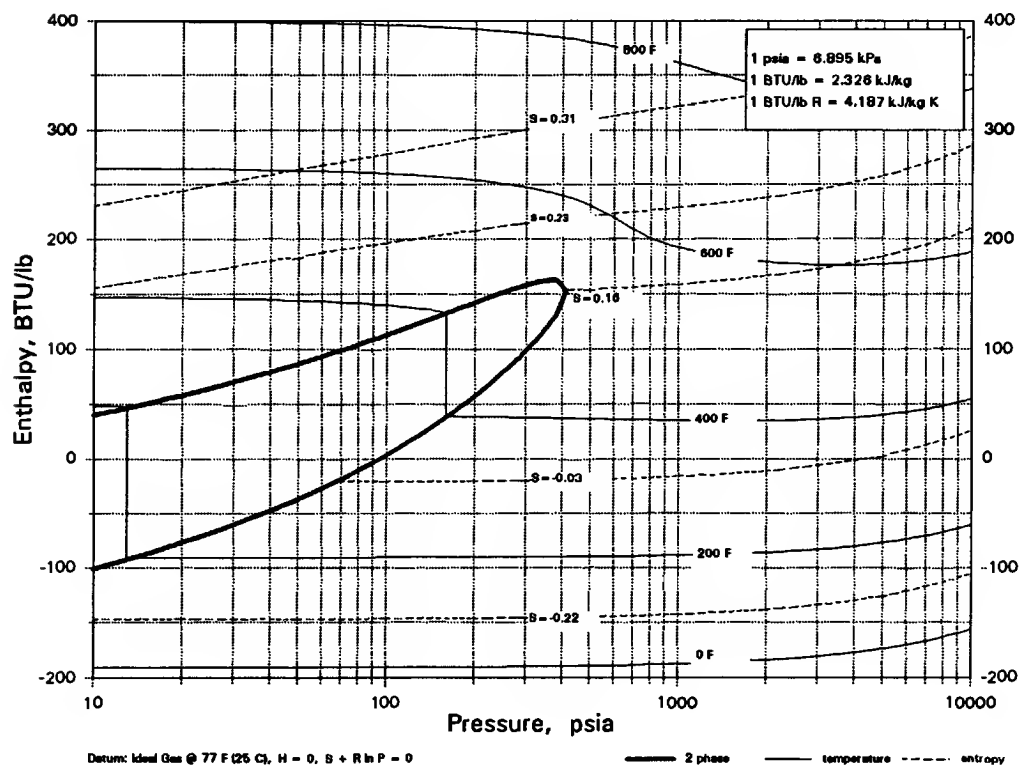
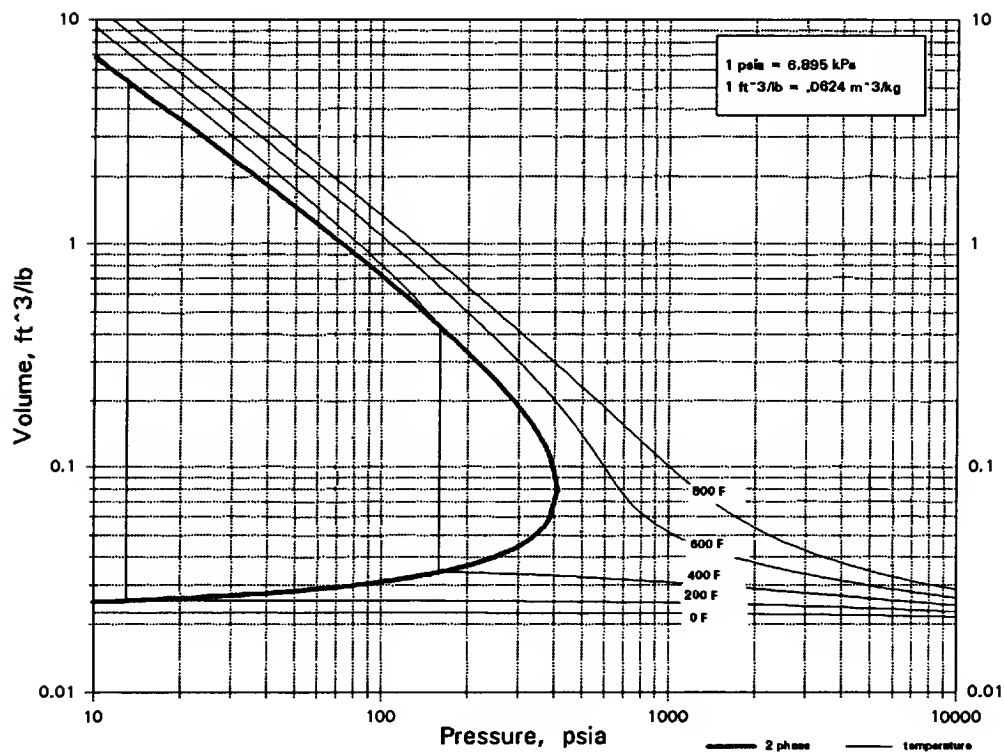


C7H14
cis-3-HEPTENE



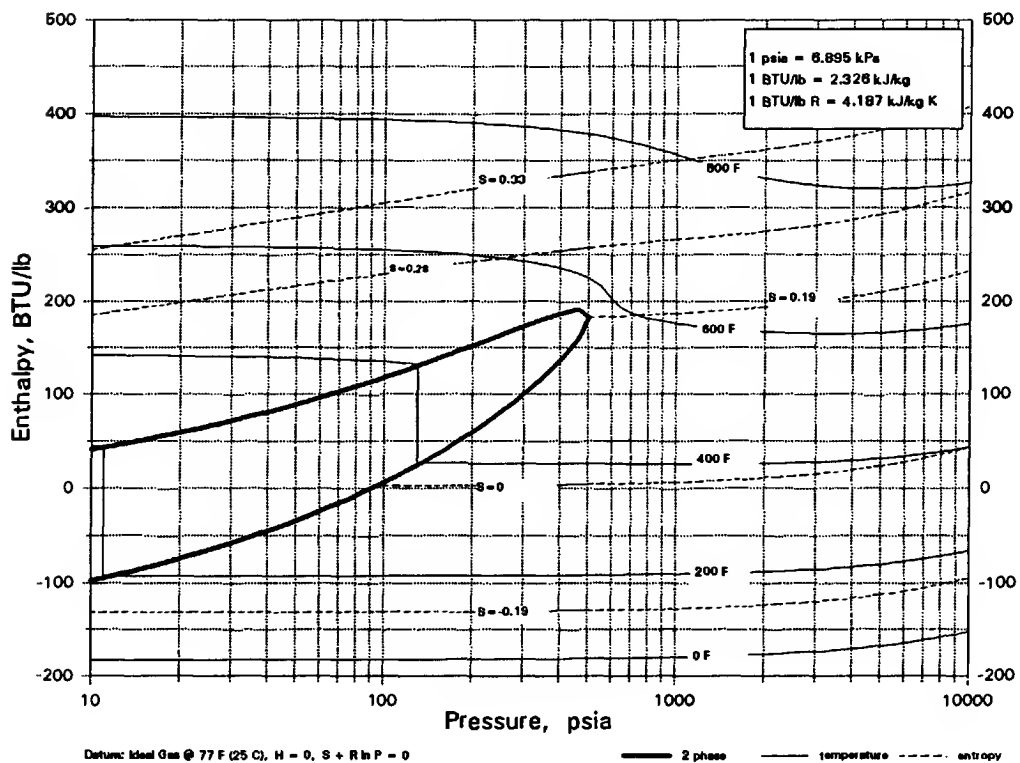
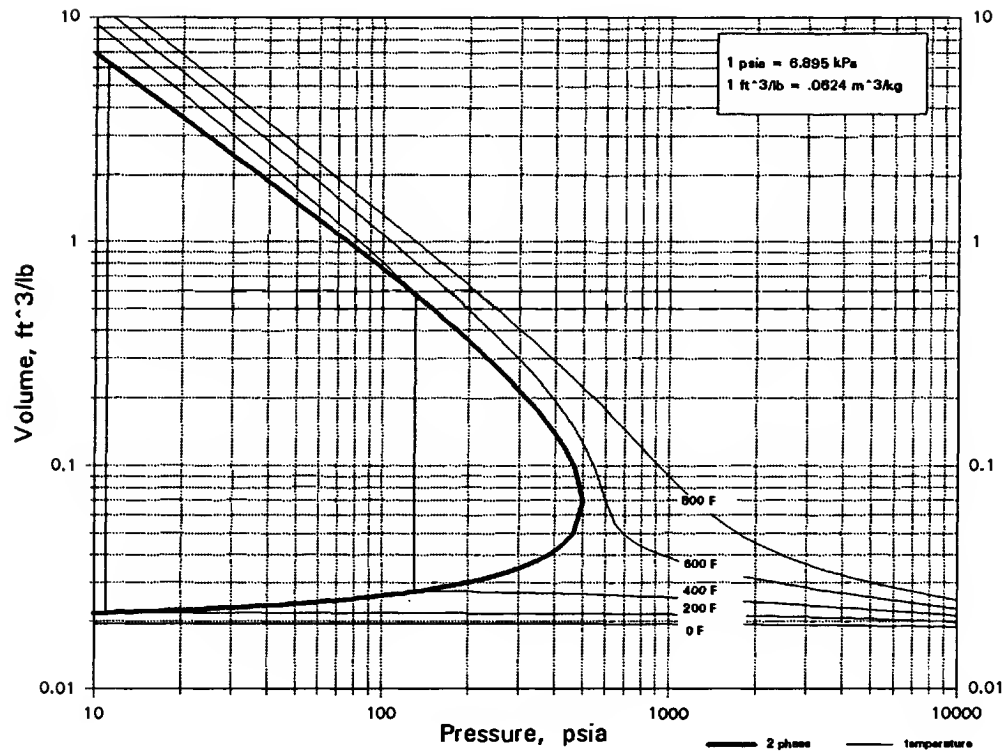
C7H14

trans-3-HEPTENE



C7H14

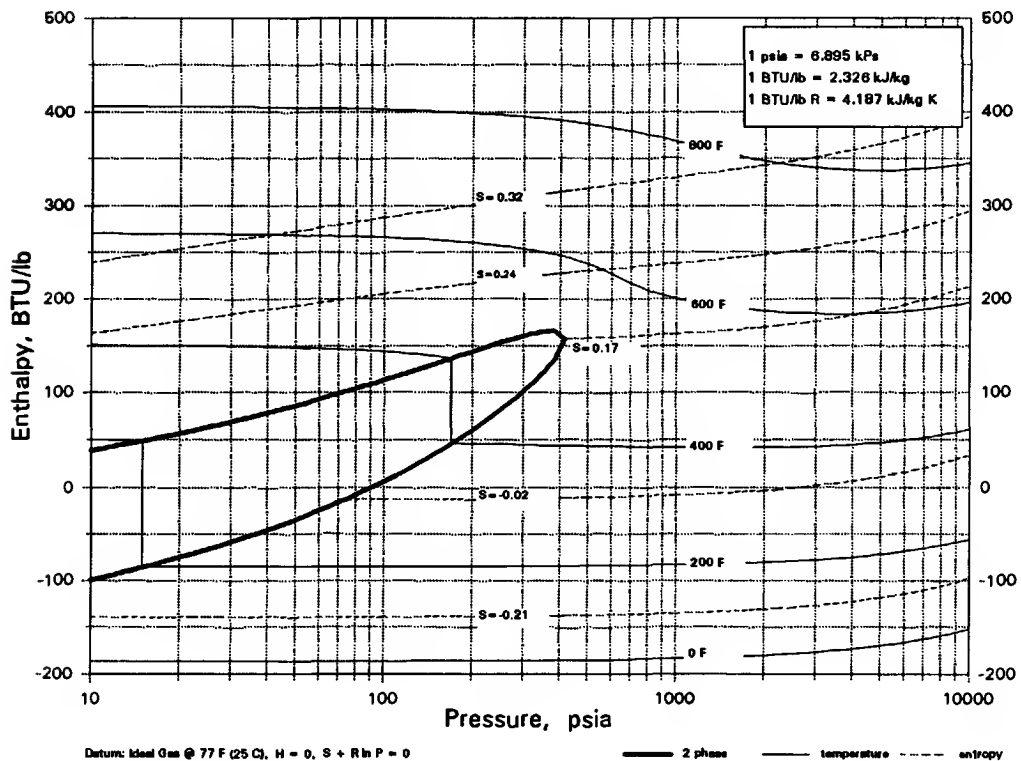
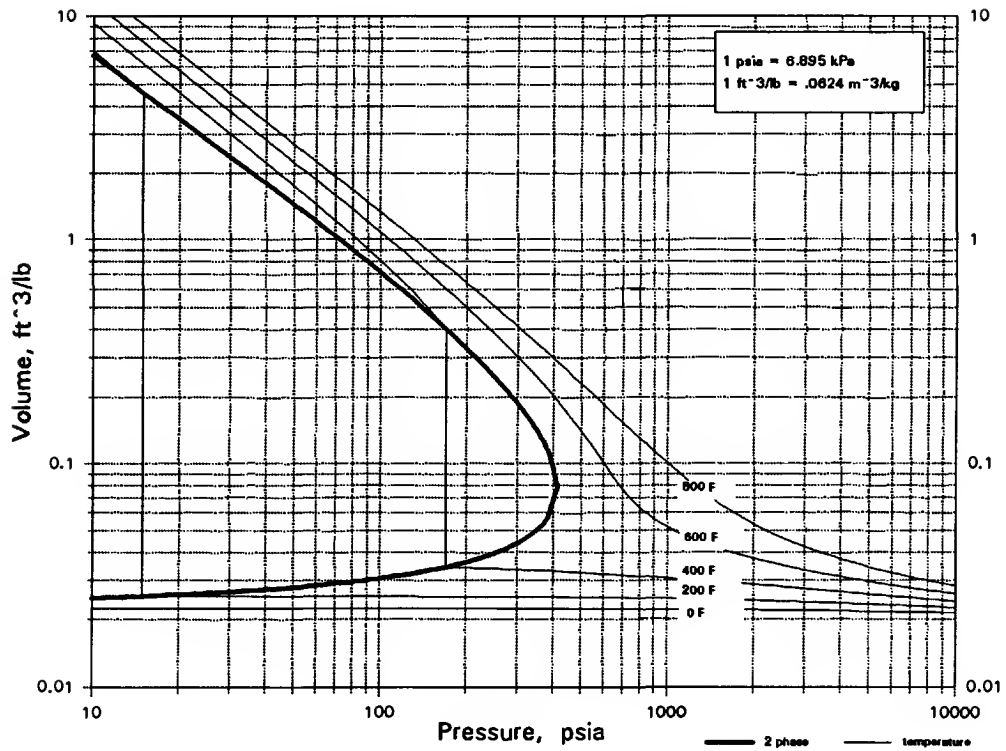
METHYLCYCLOHEXANE



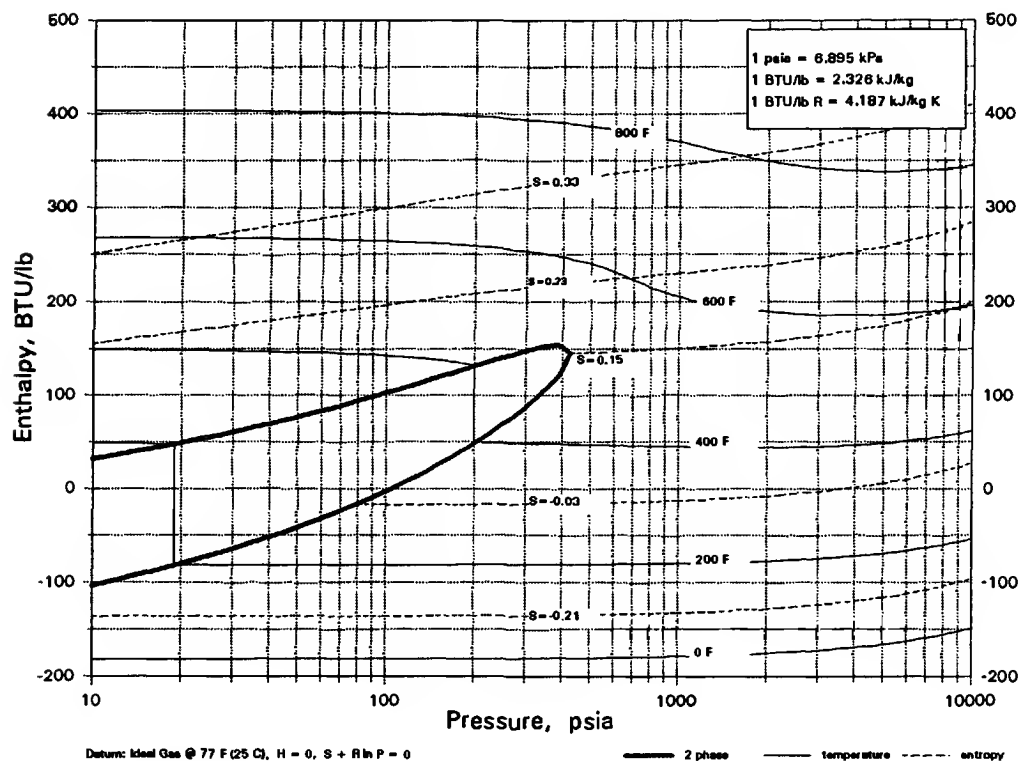
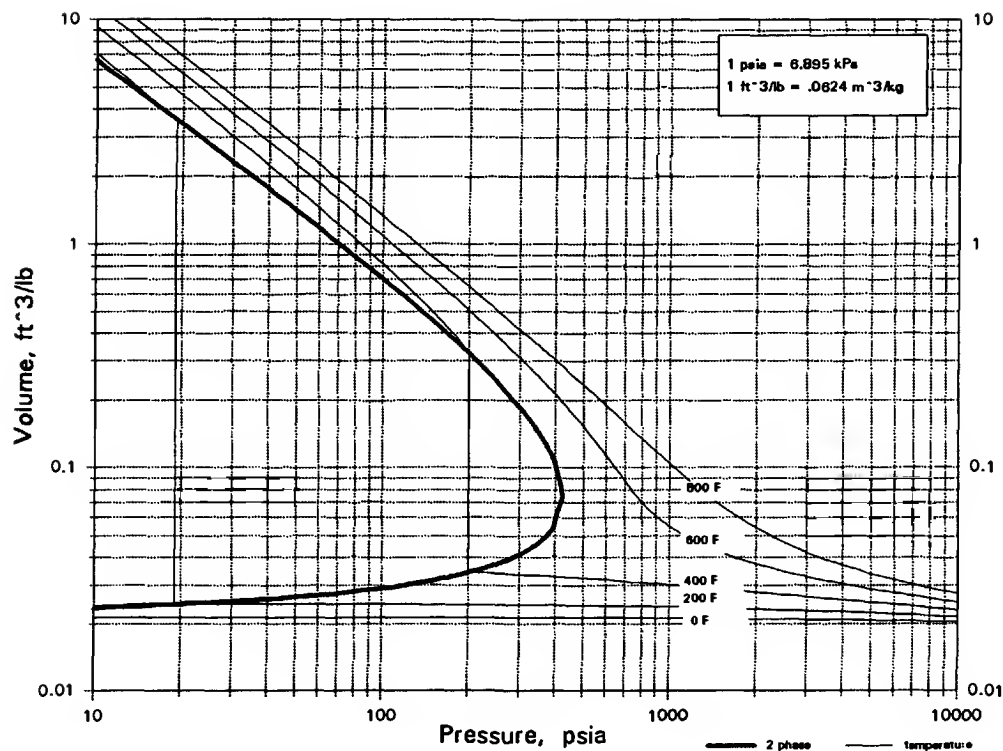
Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

C7H14

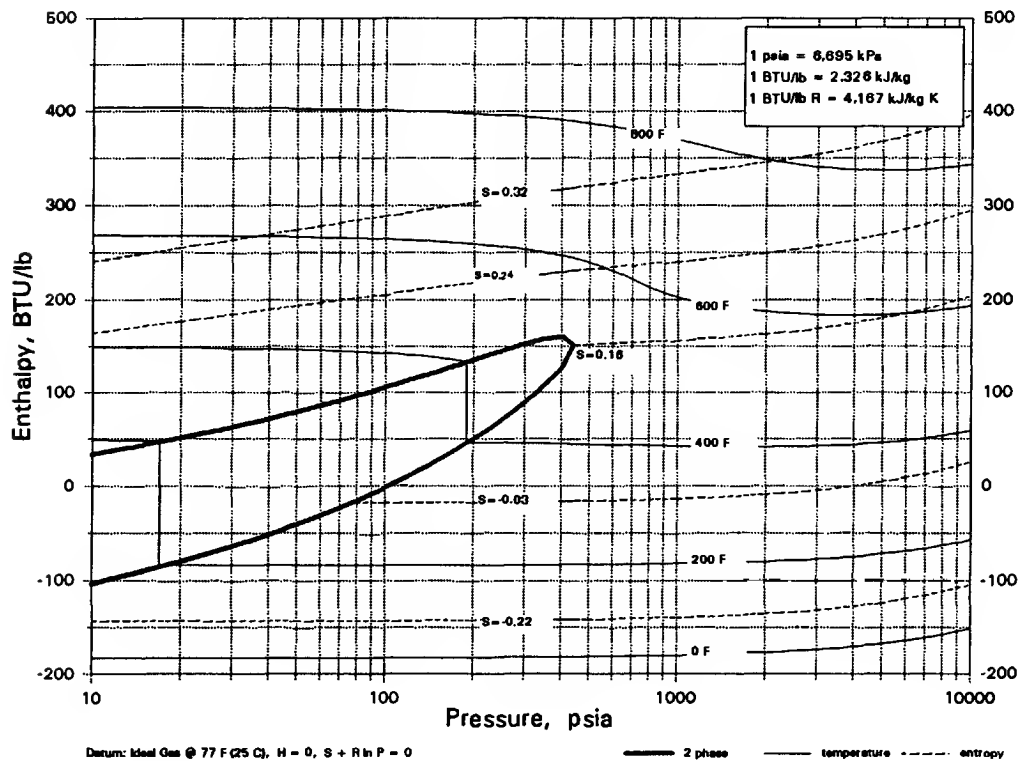
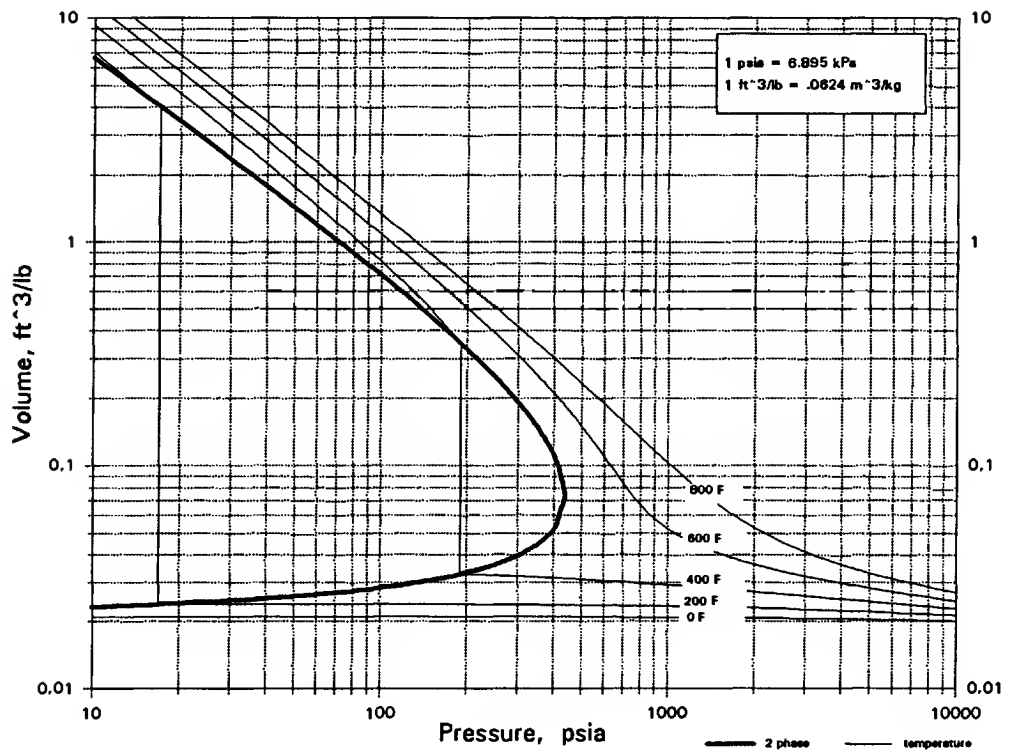
2-METHYL-1-HEXENE



C7H14
3-METHYL-1-HEXENE

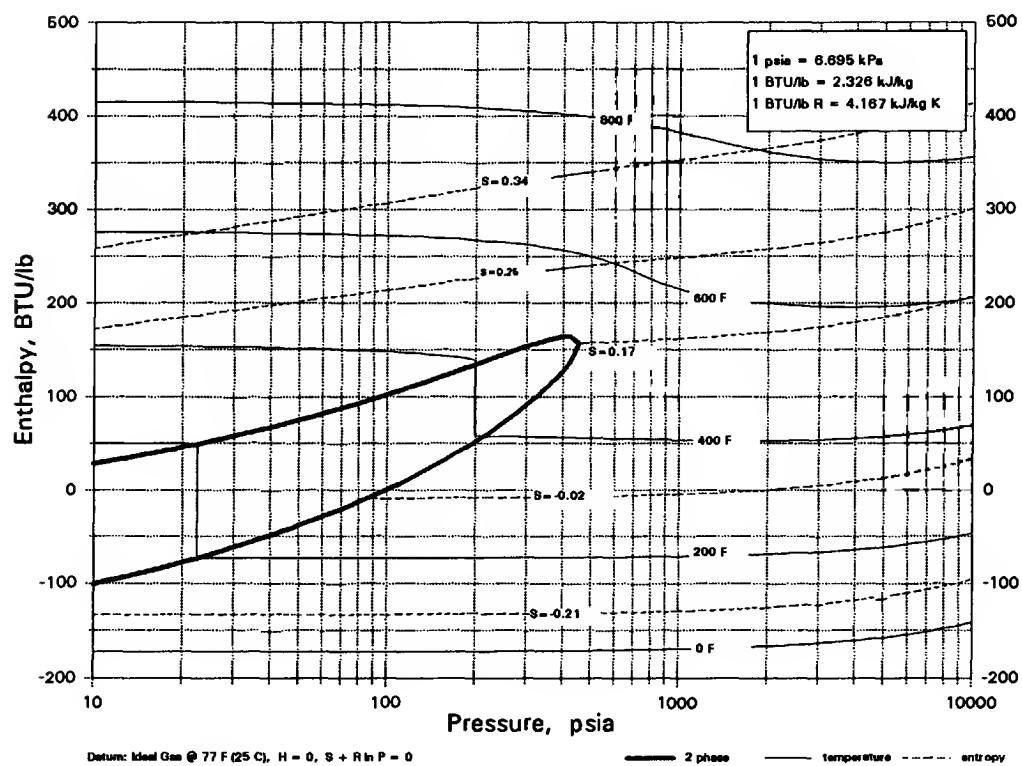
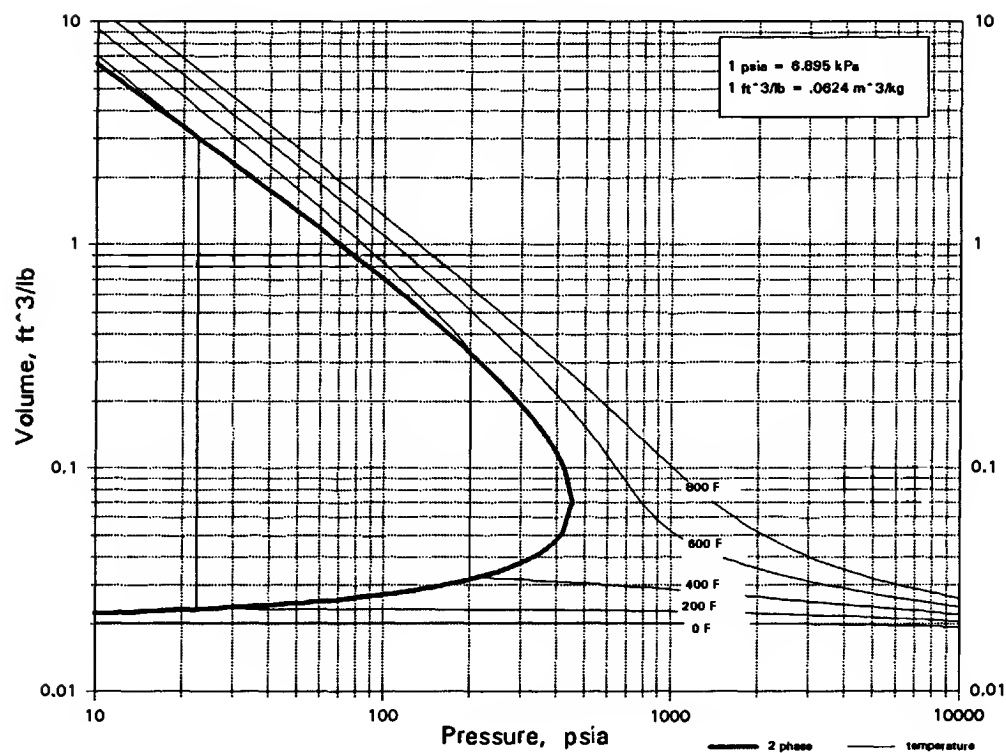


C7H14
4-METHYL-1-HEXENE



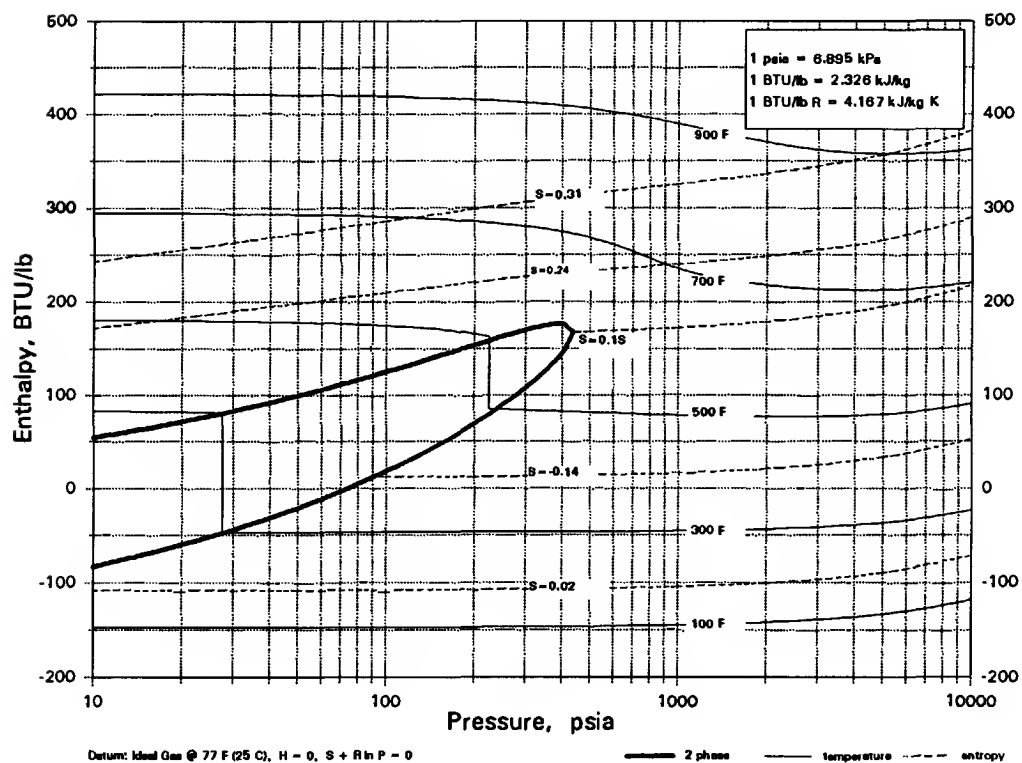
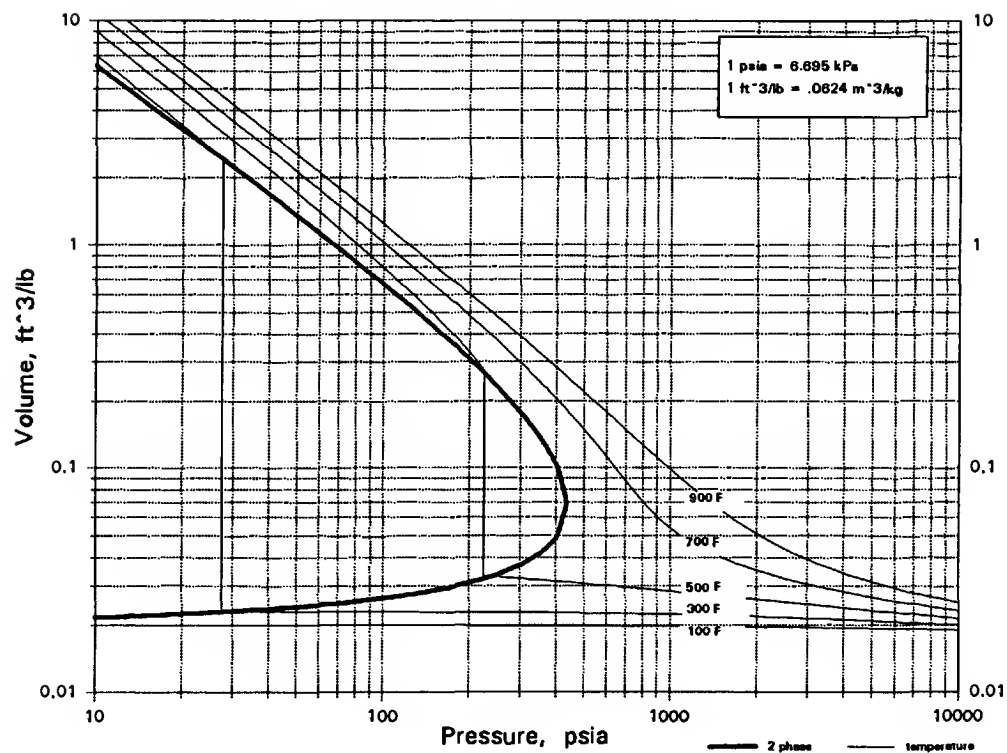
C7H14

2-3-3-TRIMETHYL-1-BUTENE



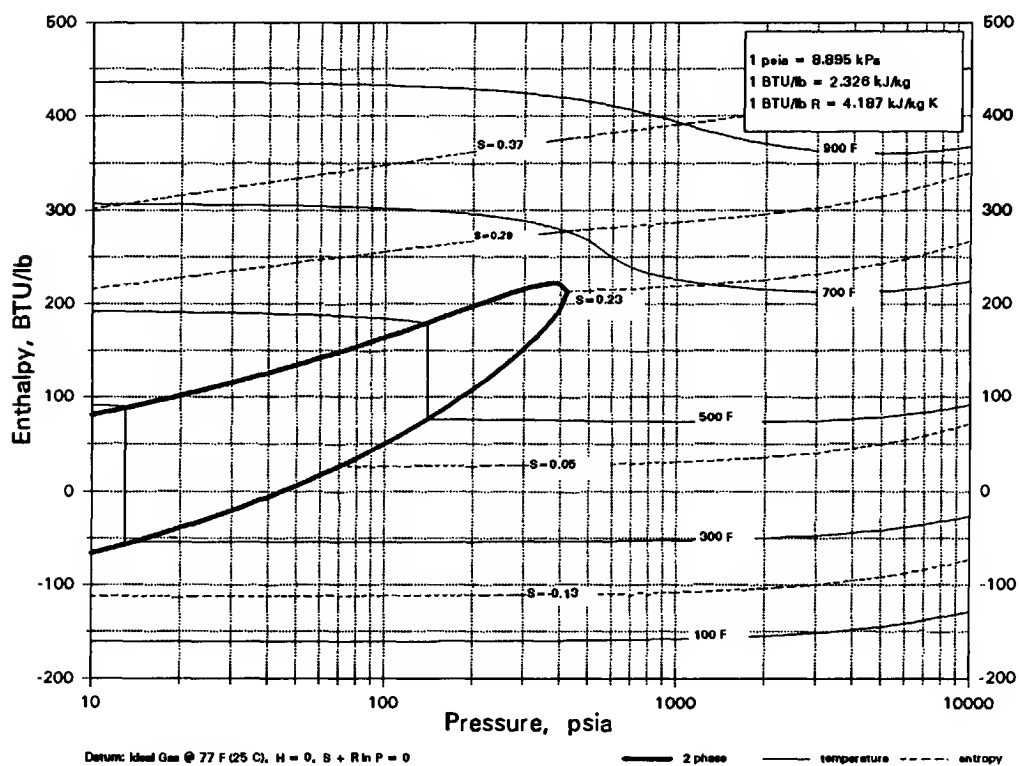
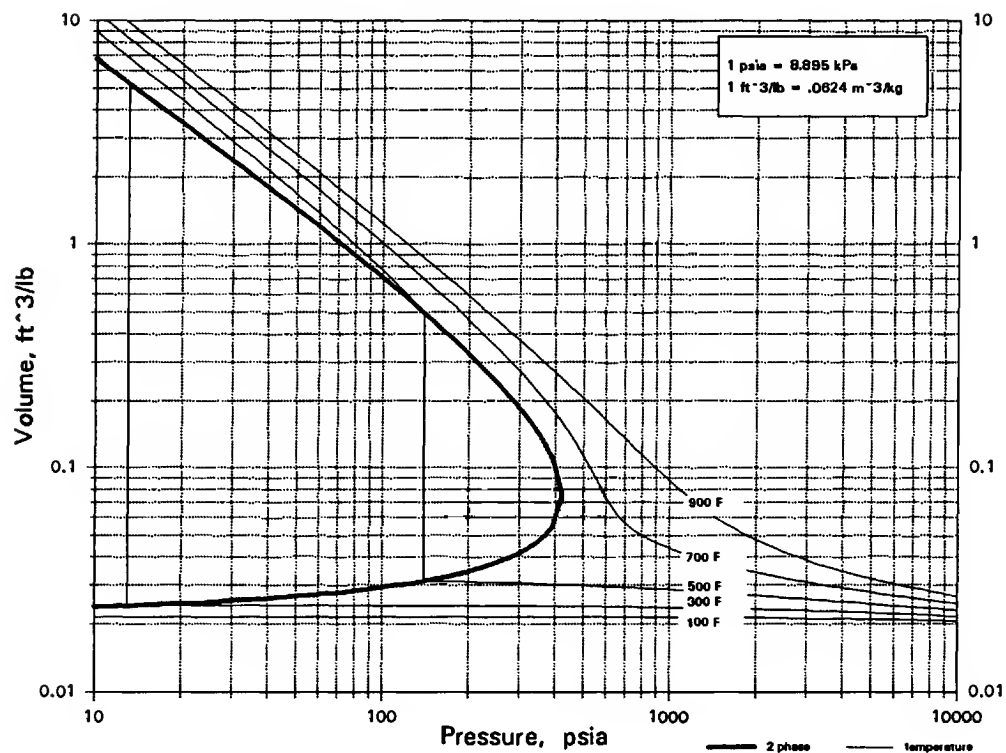
C7H14O

DIISOPROPYL KETONE

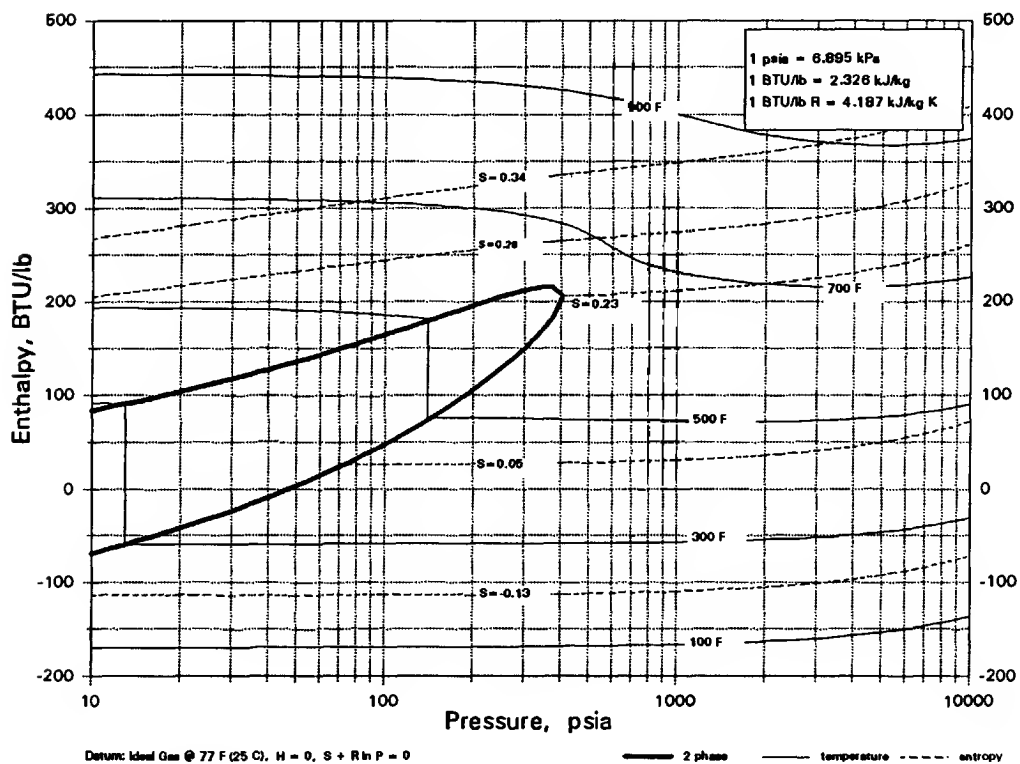
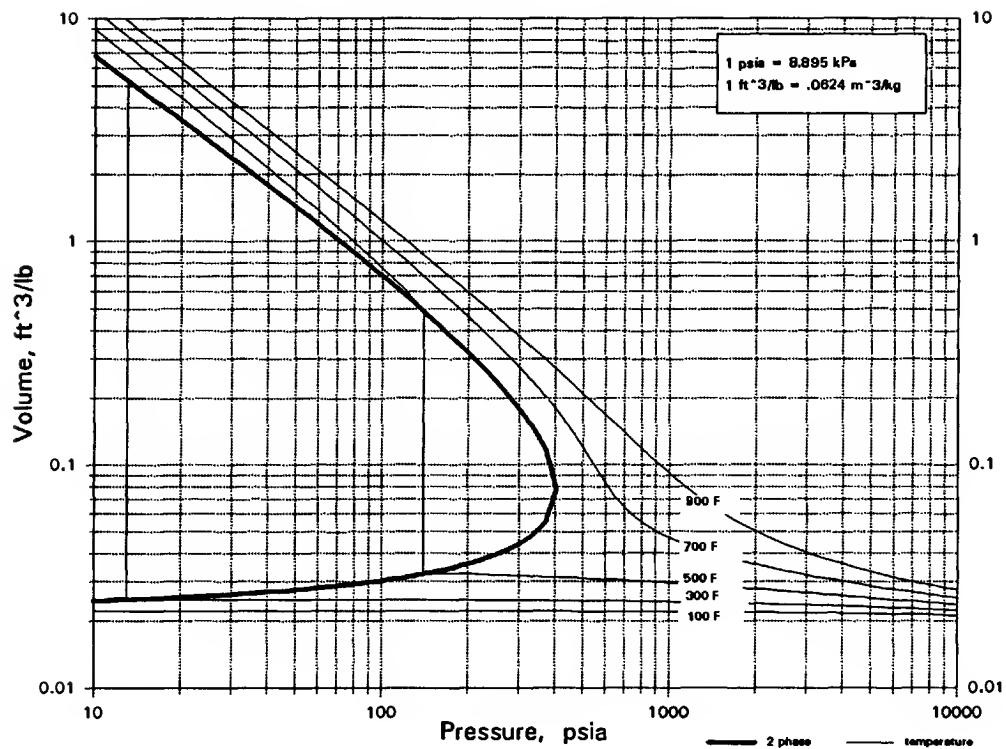


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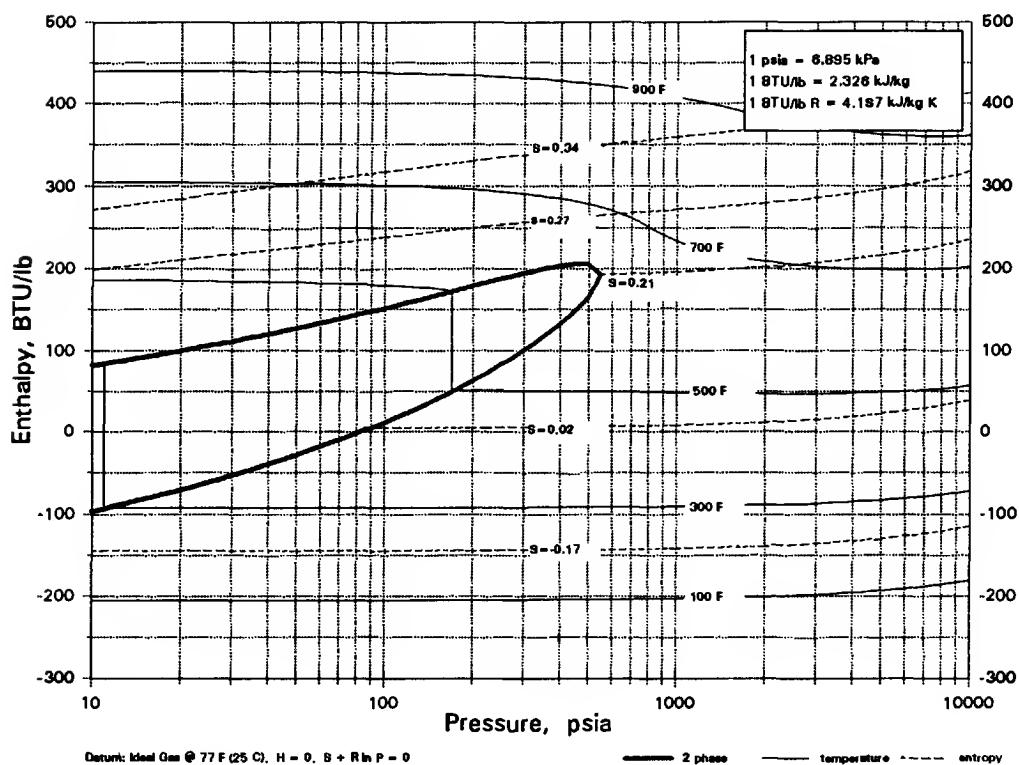
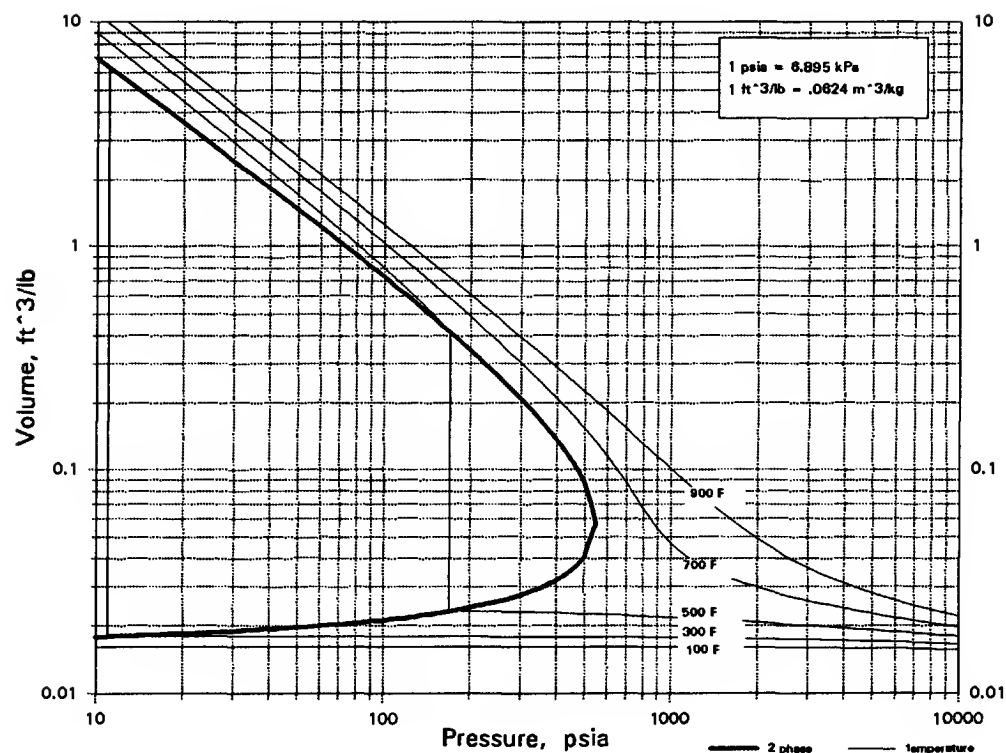


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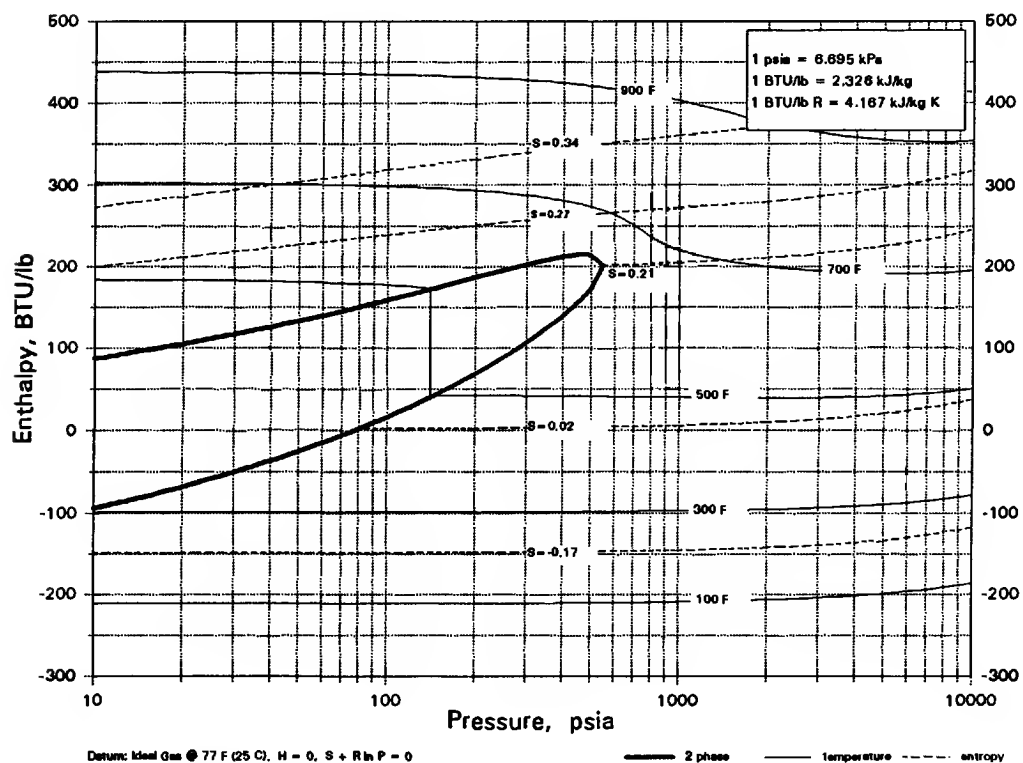
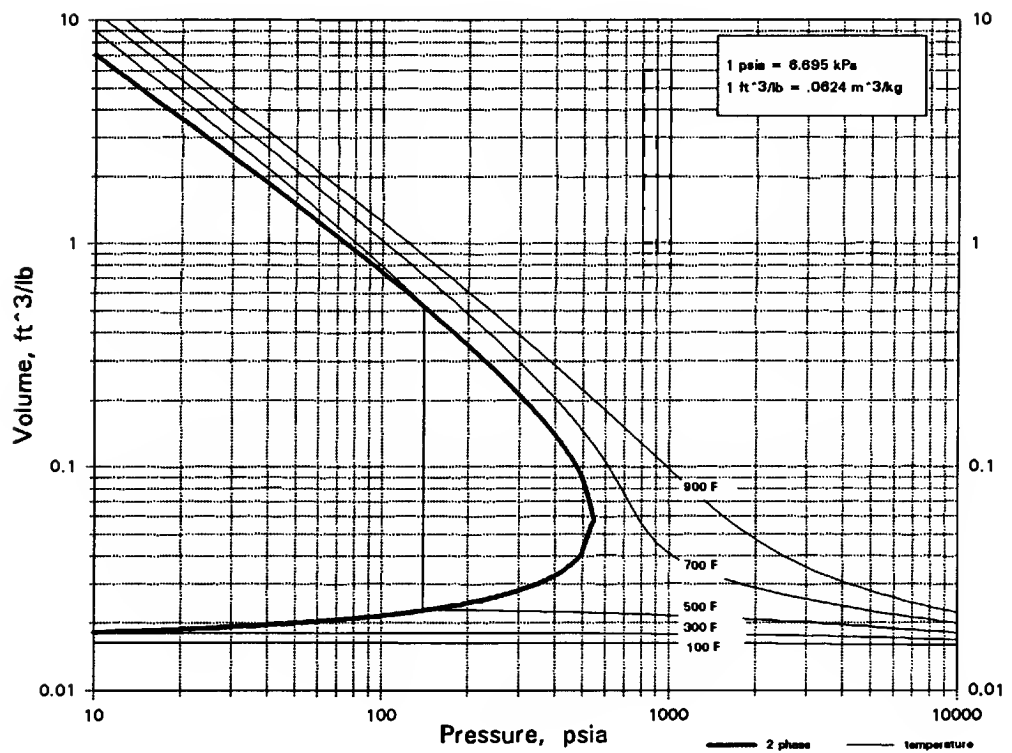
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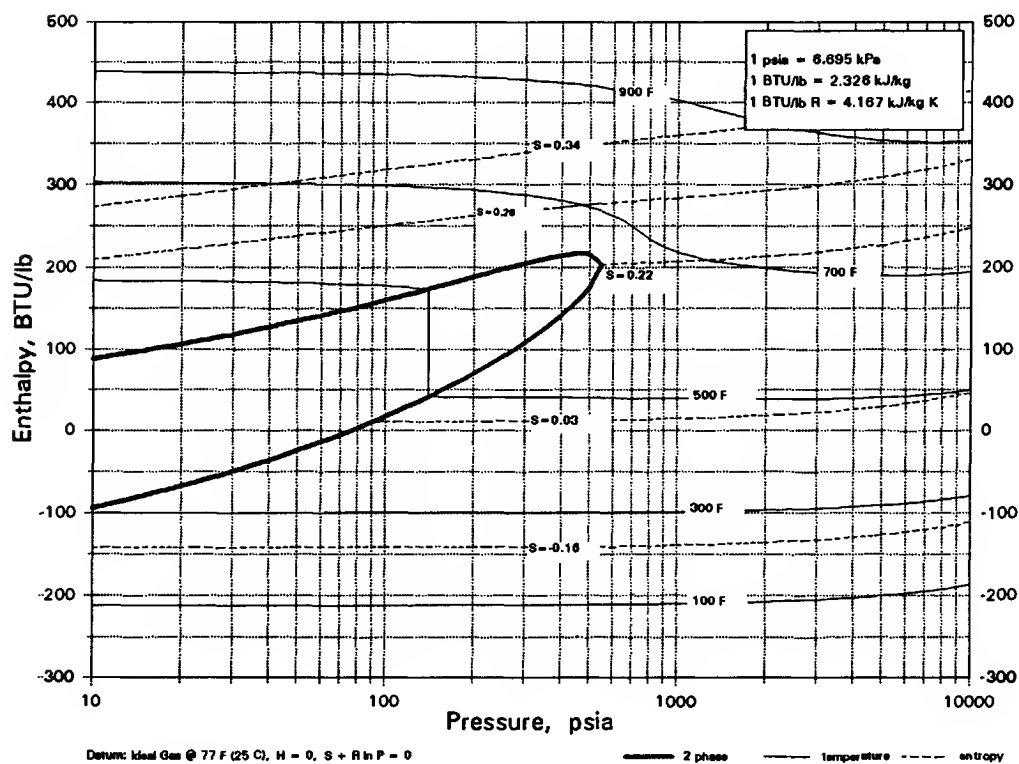
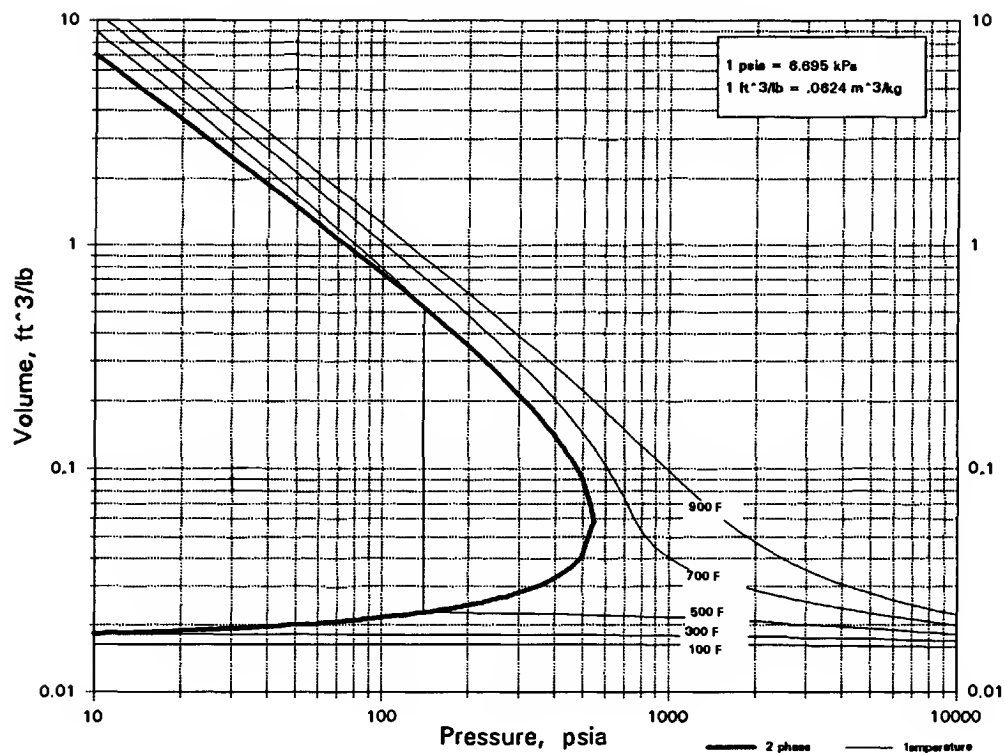
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C7H14O
cis-2-METHYLCYCLOHEXANOL



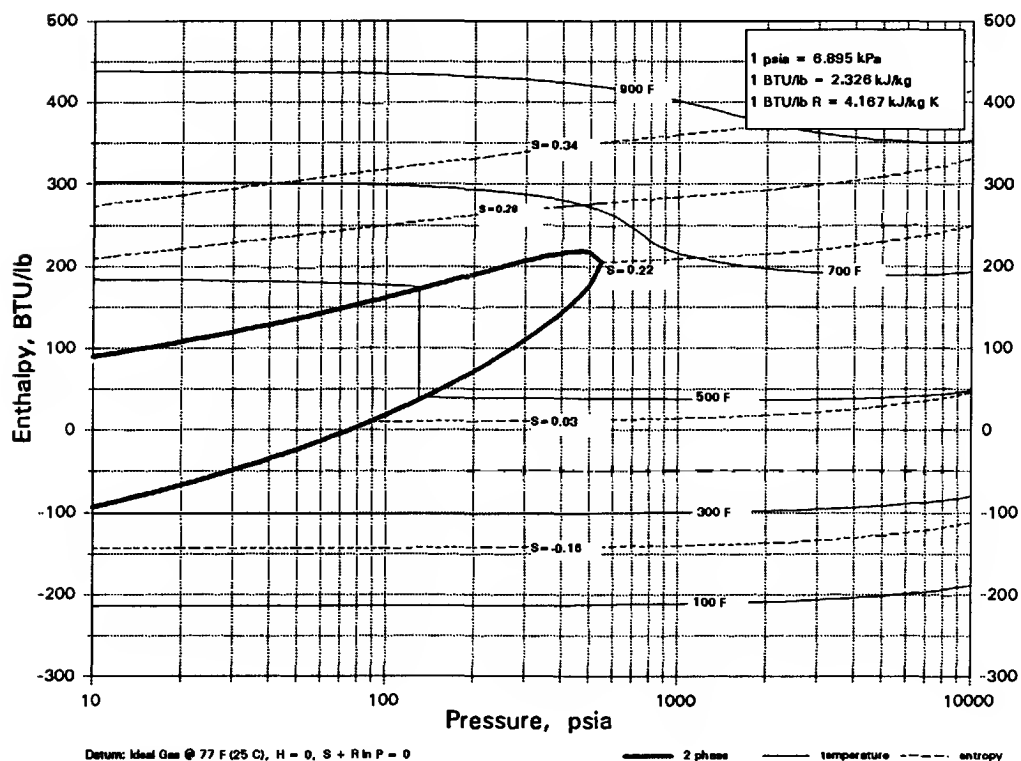
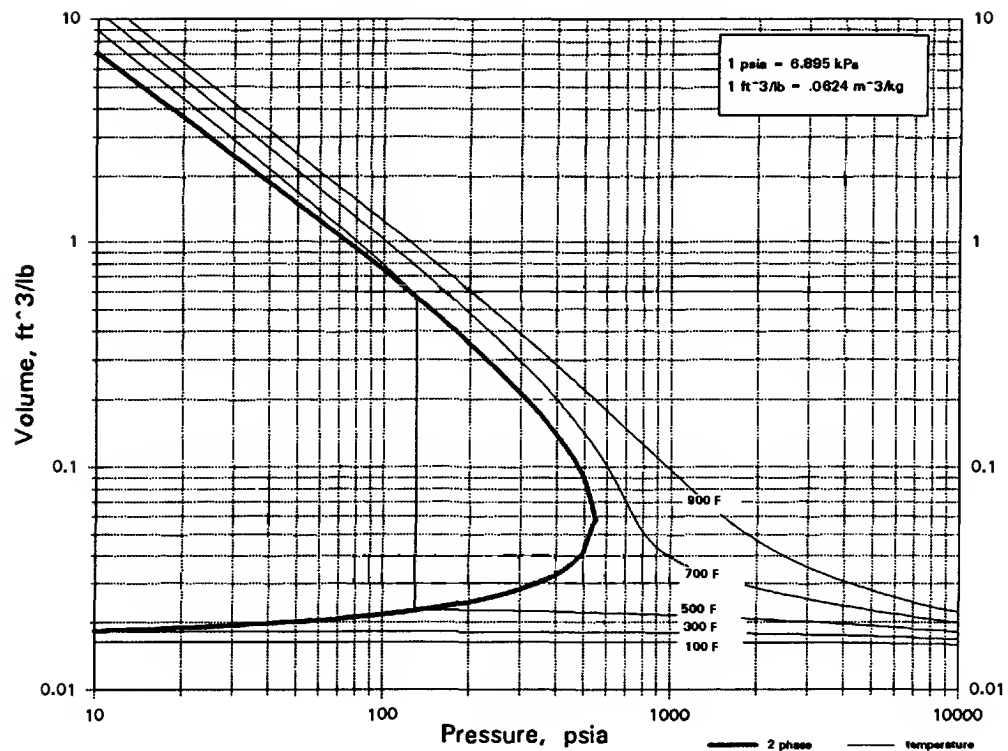
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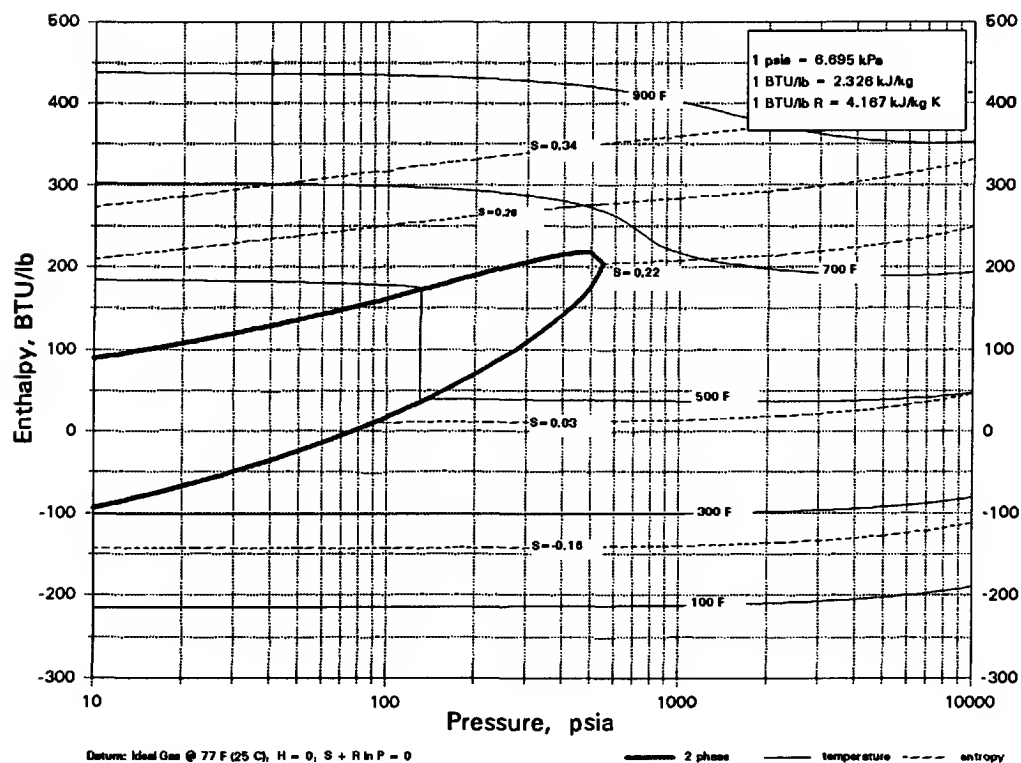
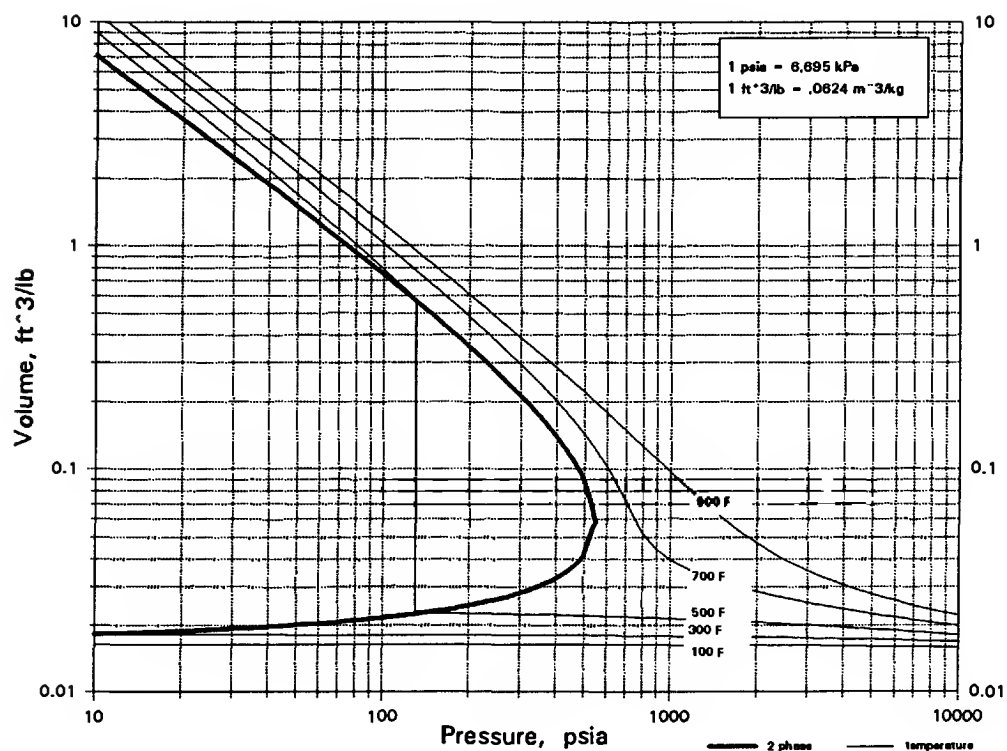
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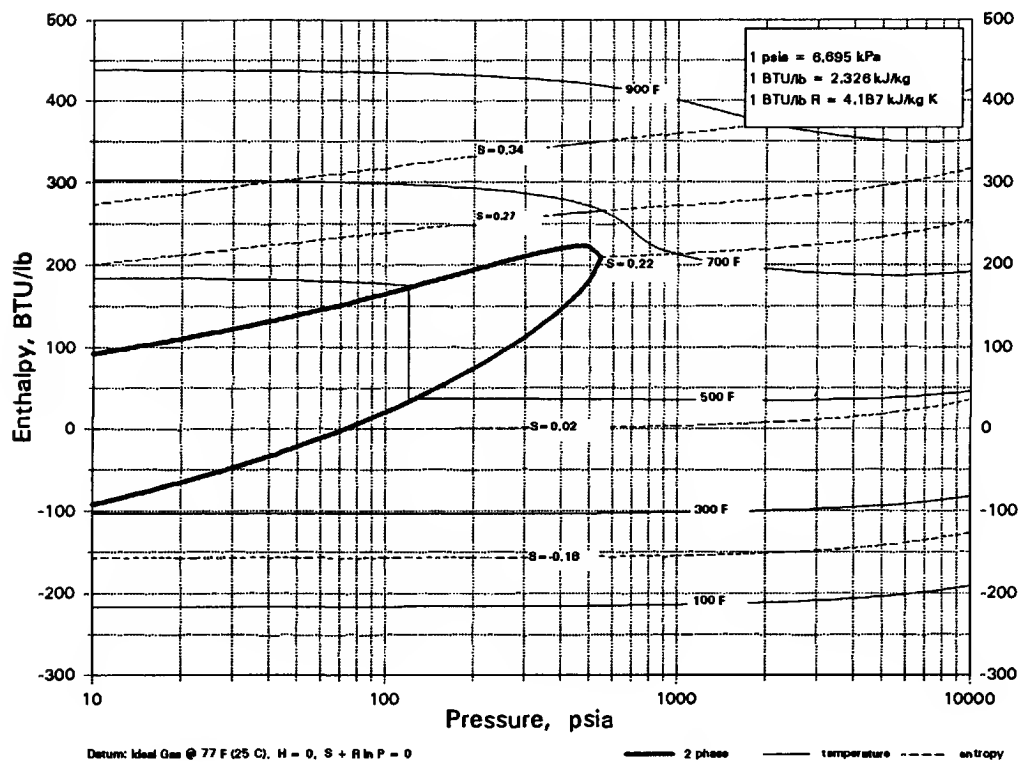
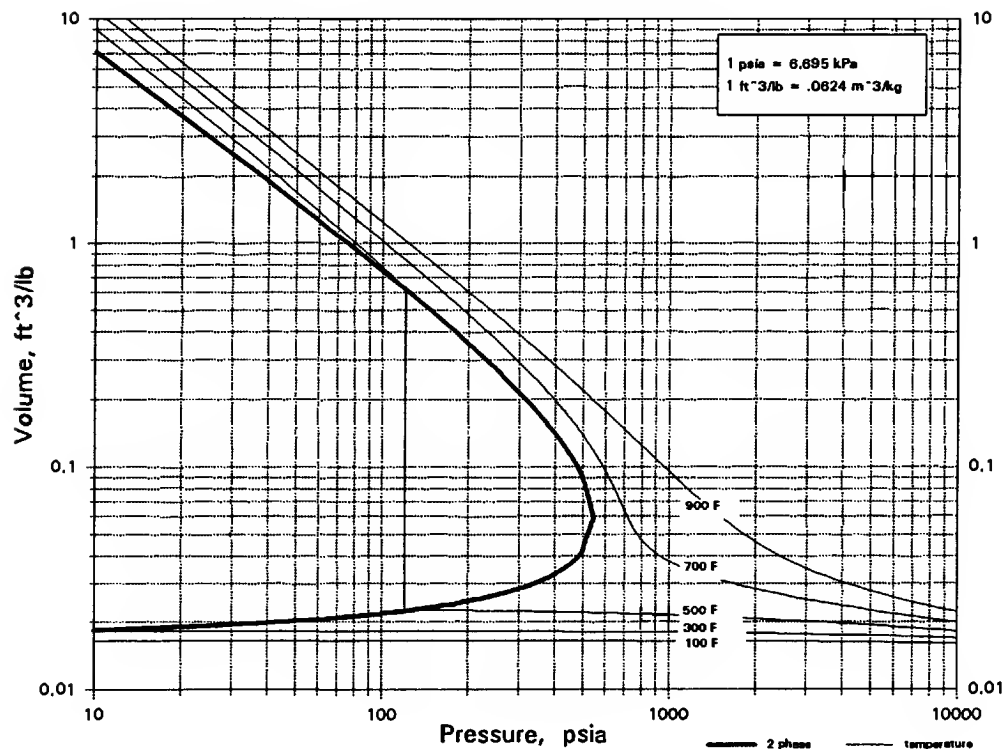
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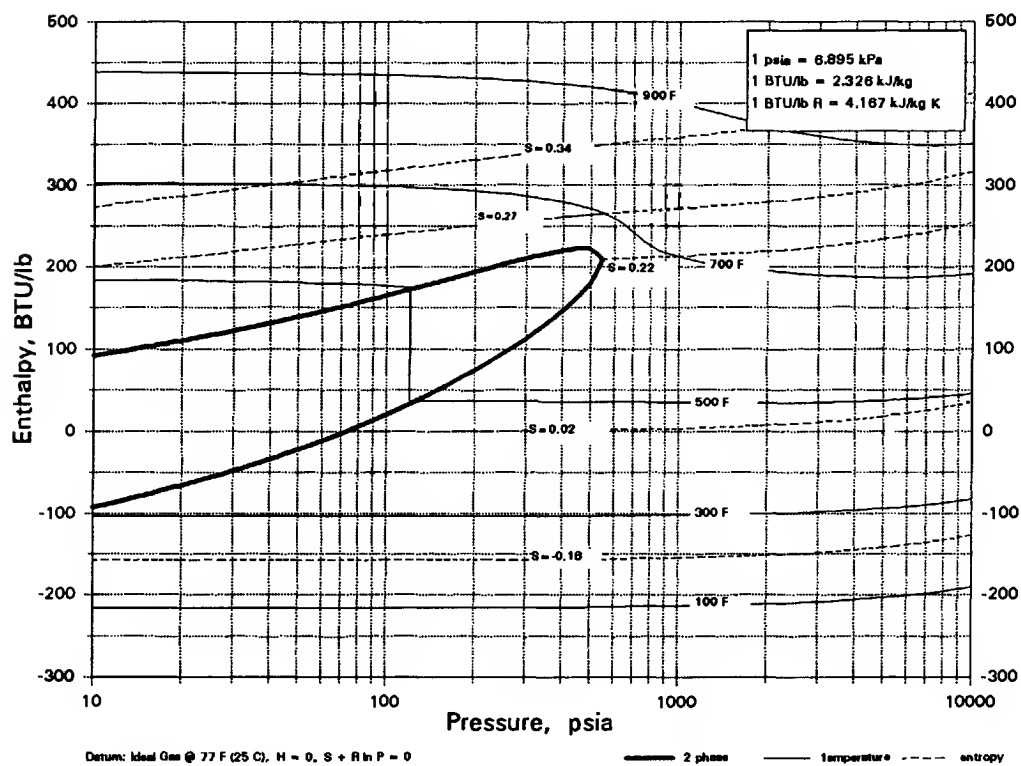
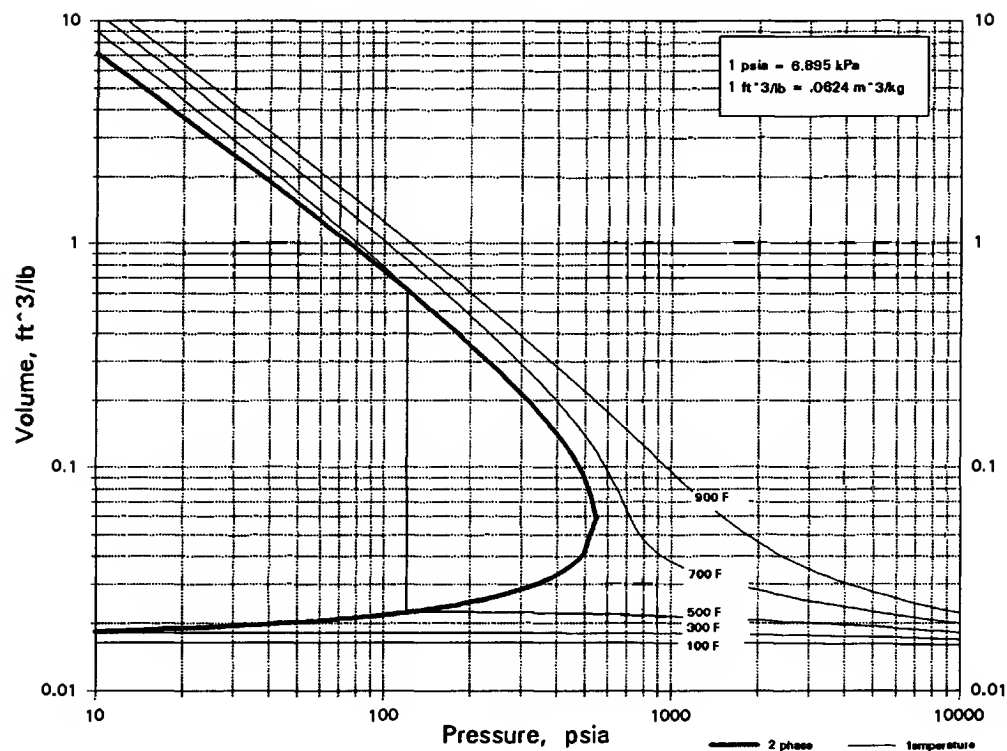
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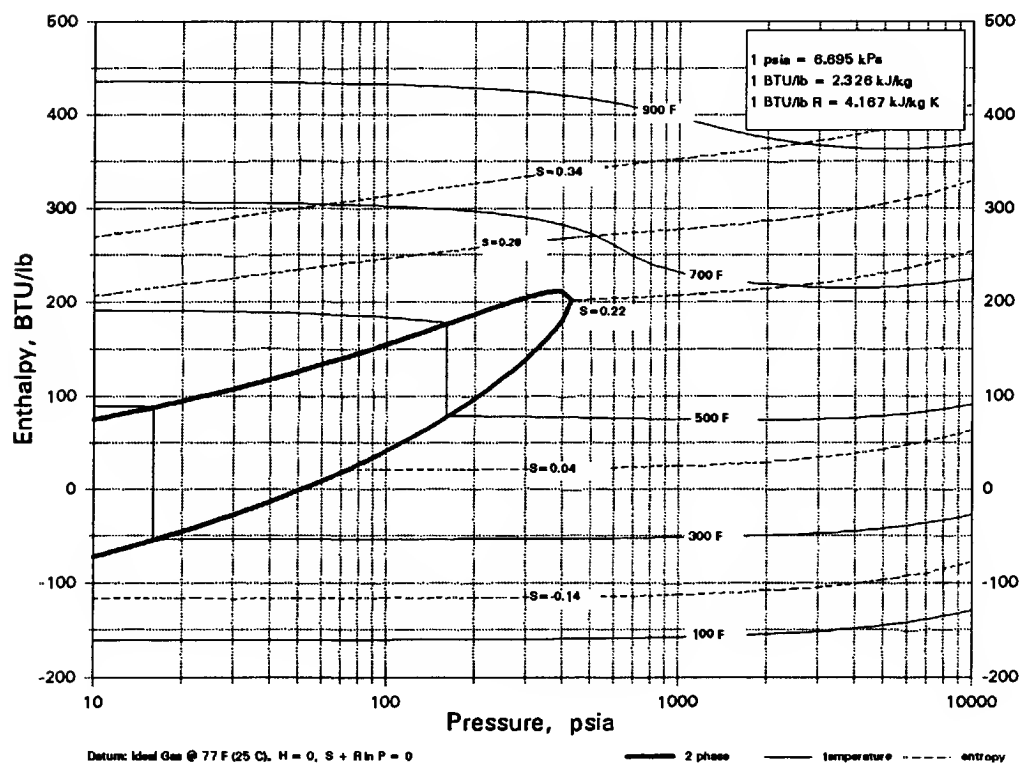
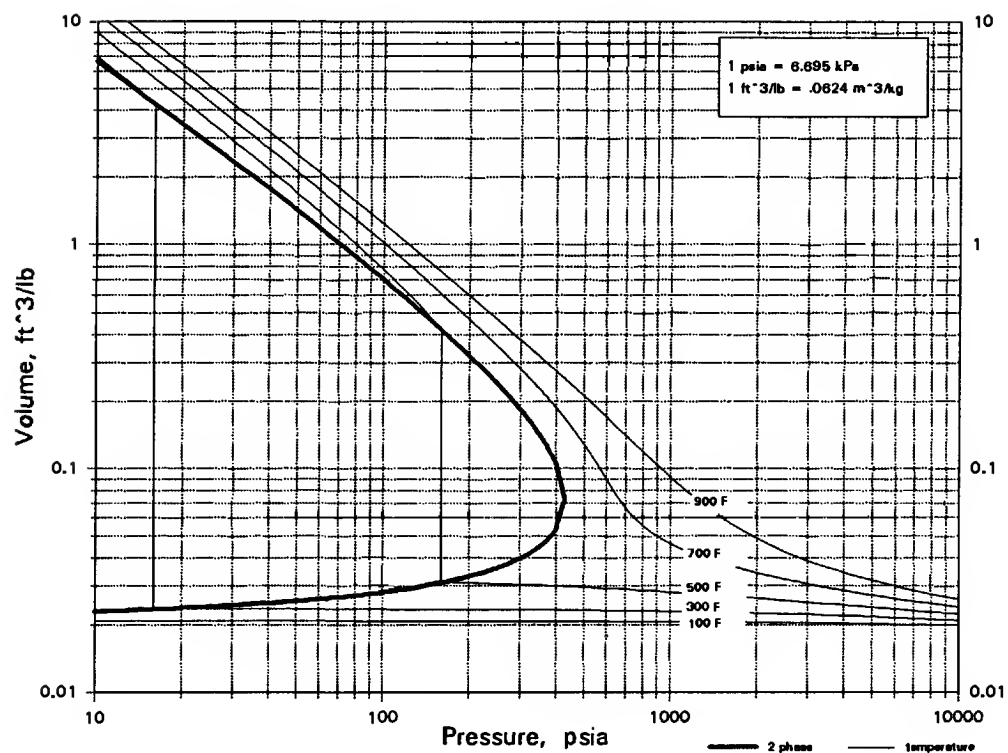
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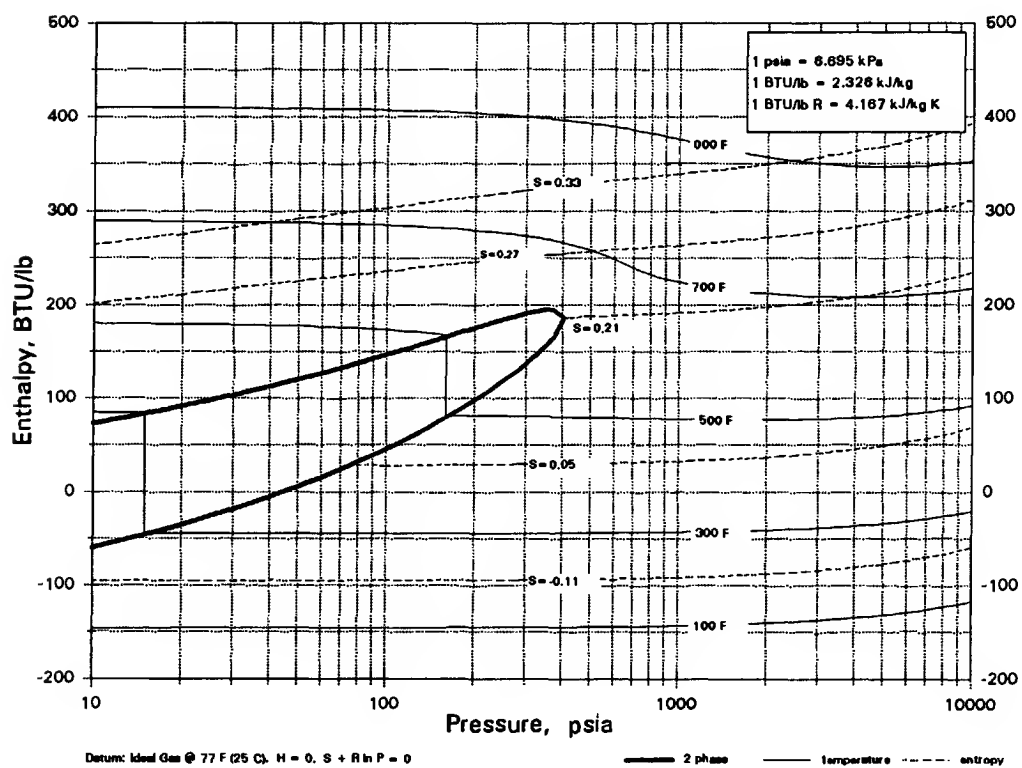
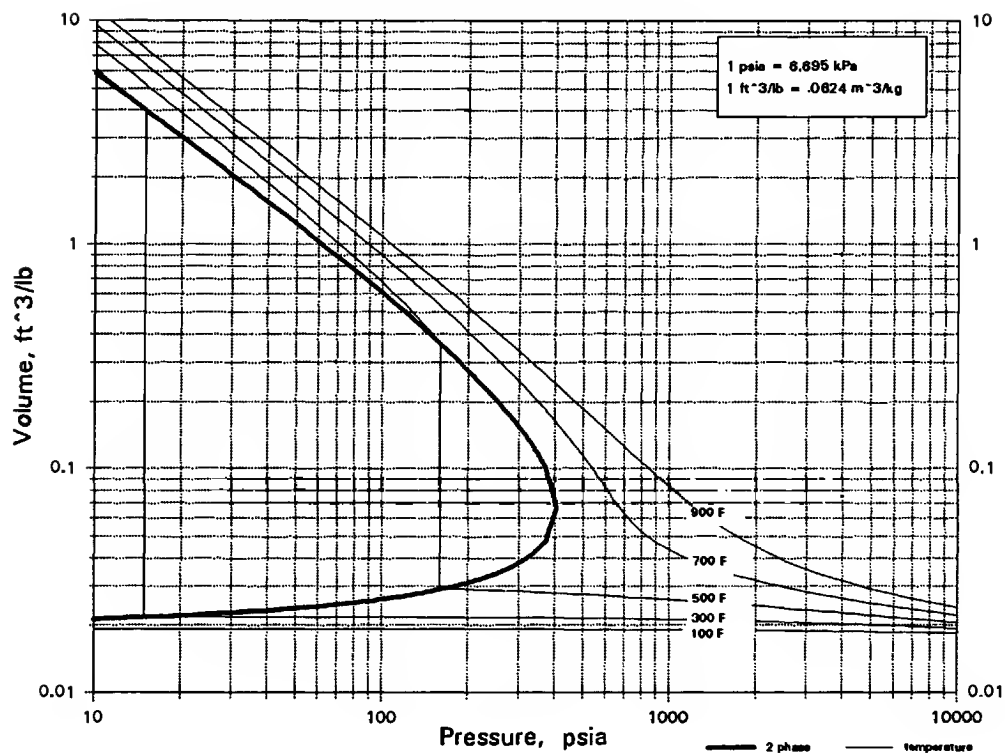
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5-METHYL-2-HEXANONE



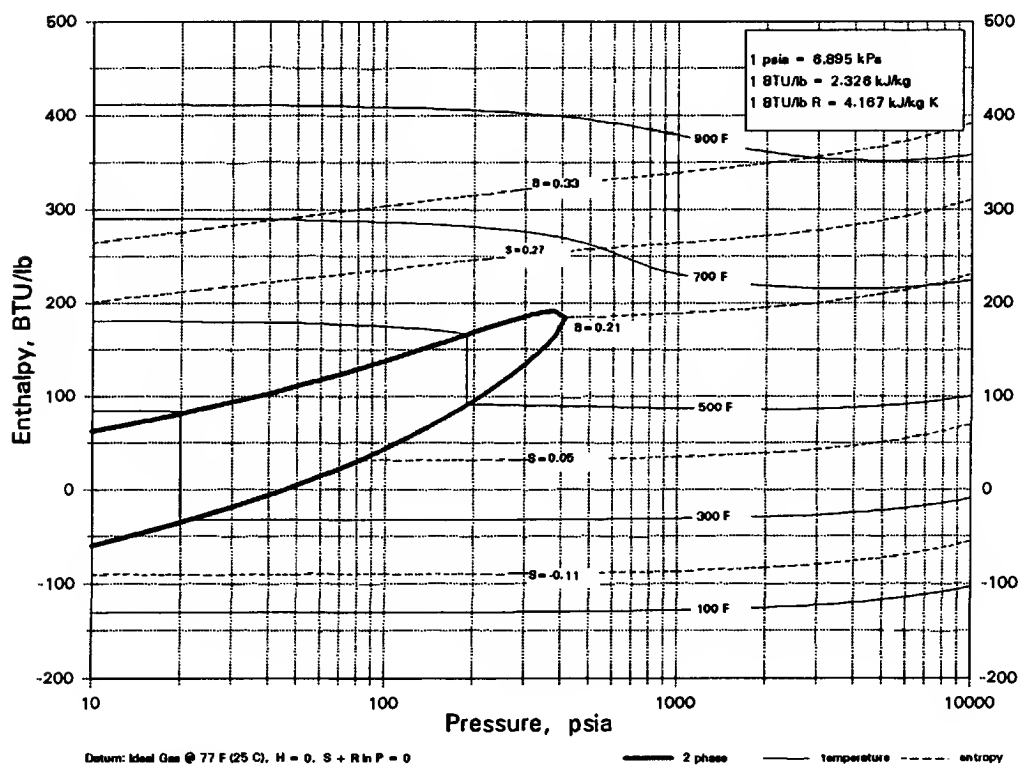
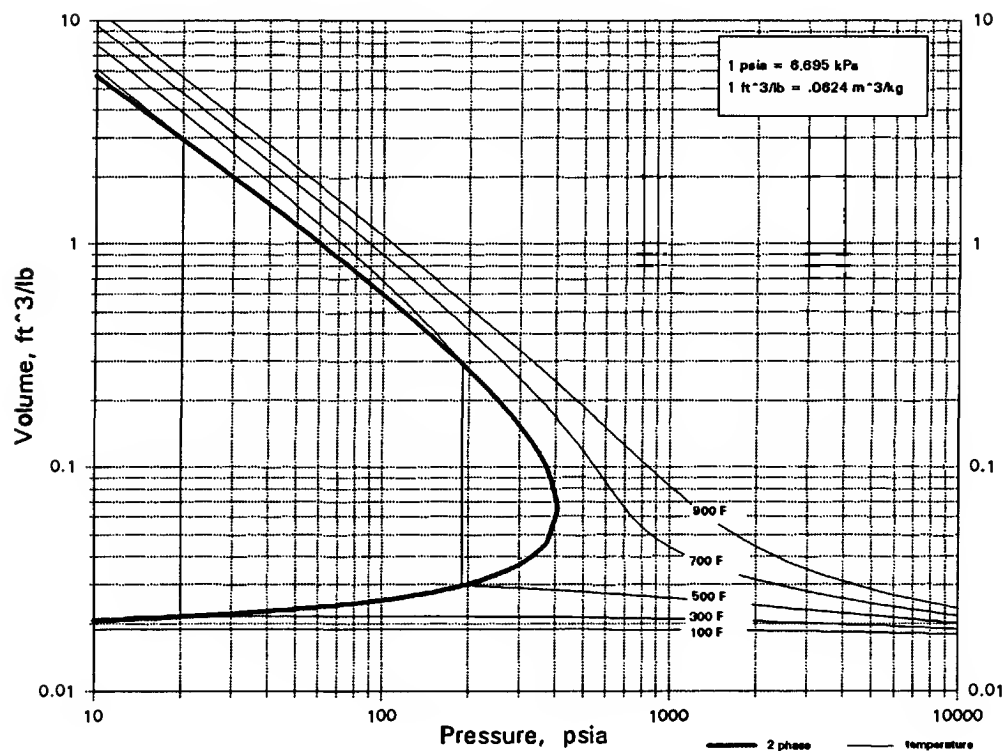
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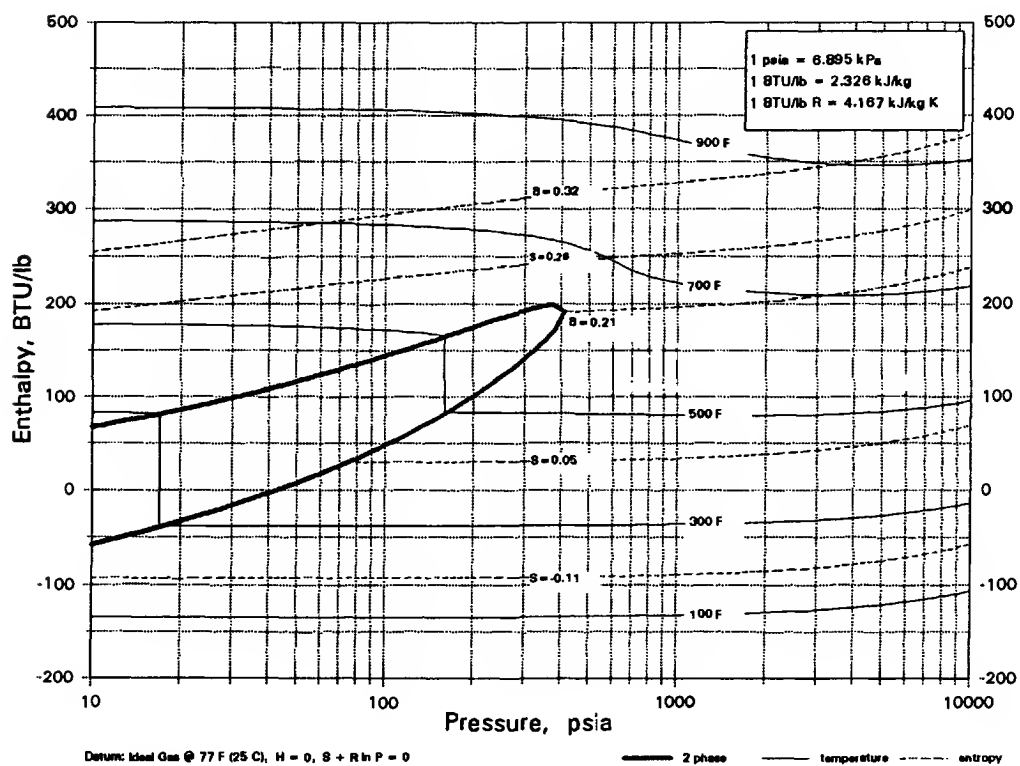
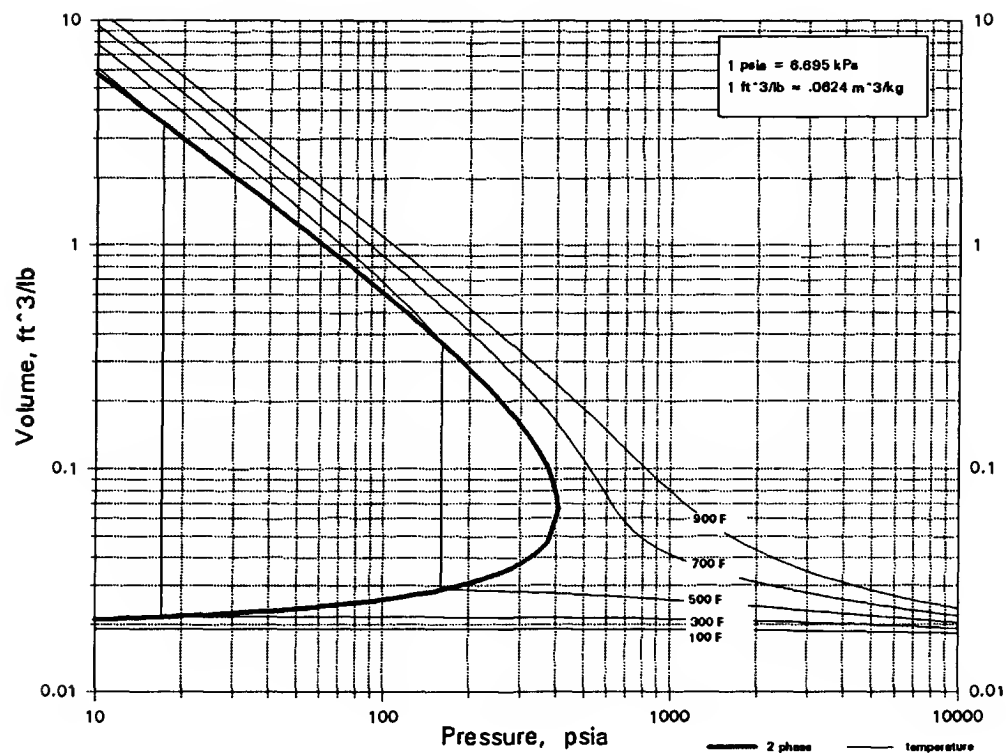
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ETHYL ISOVALERATE



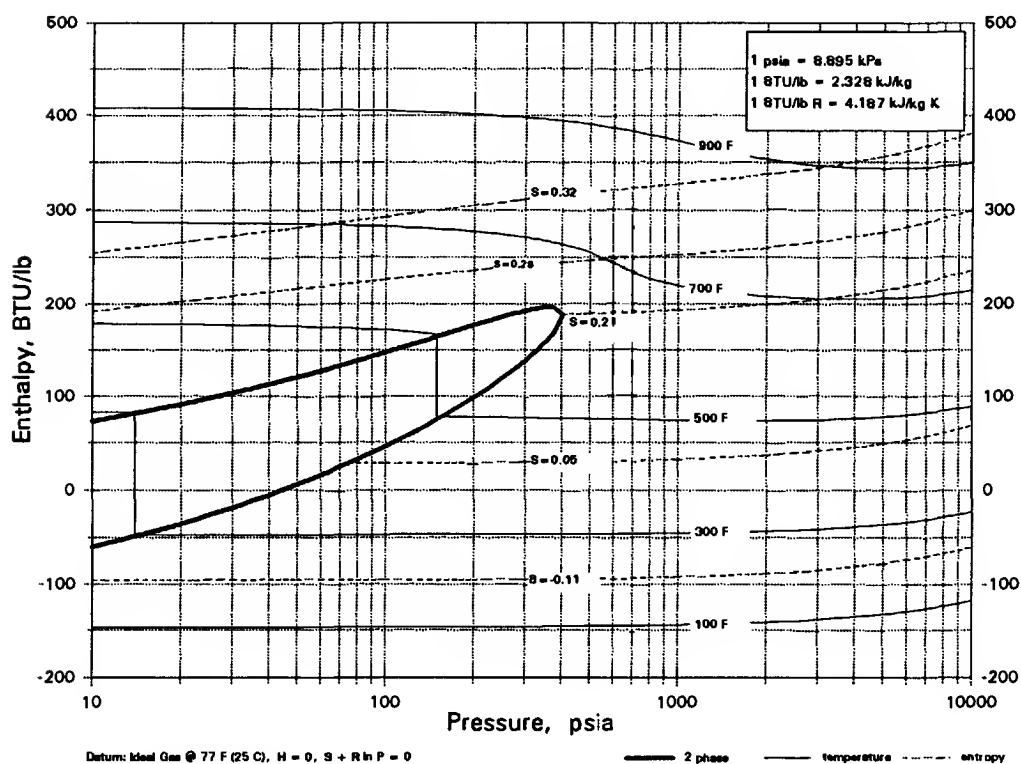
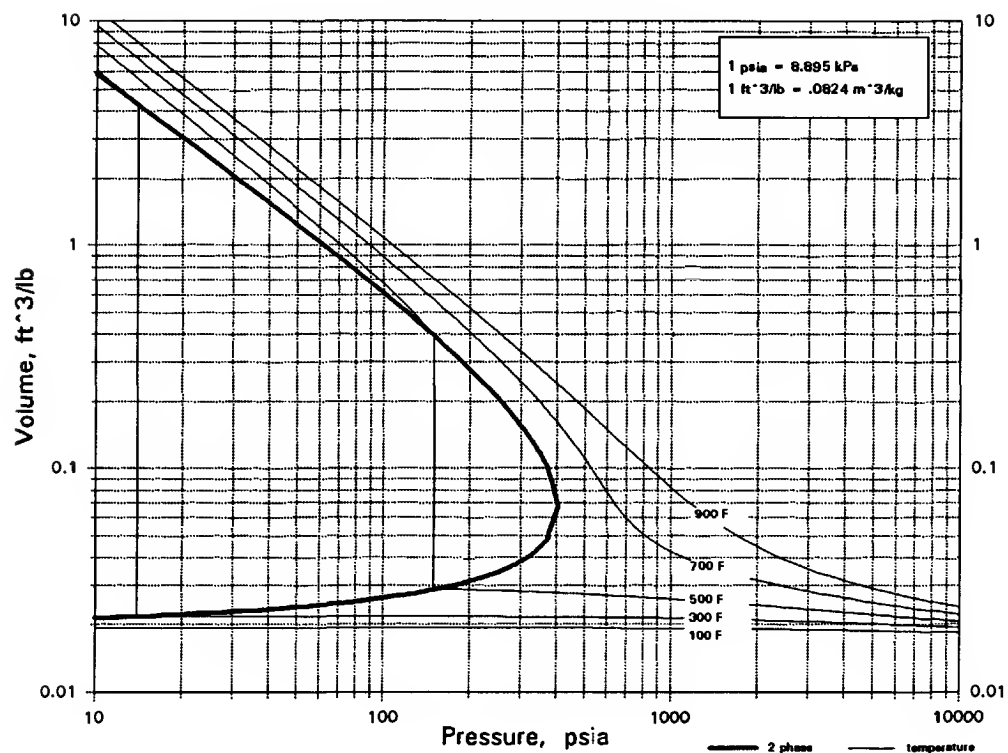
C7H14O2

ISOPENTYL ACETATE



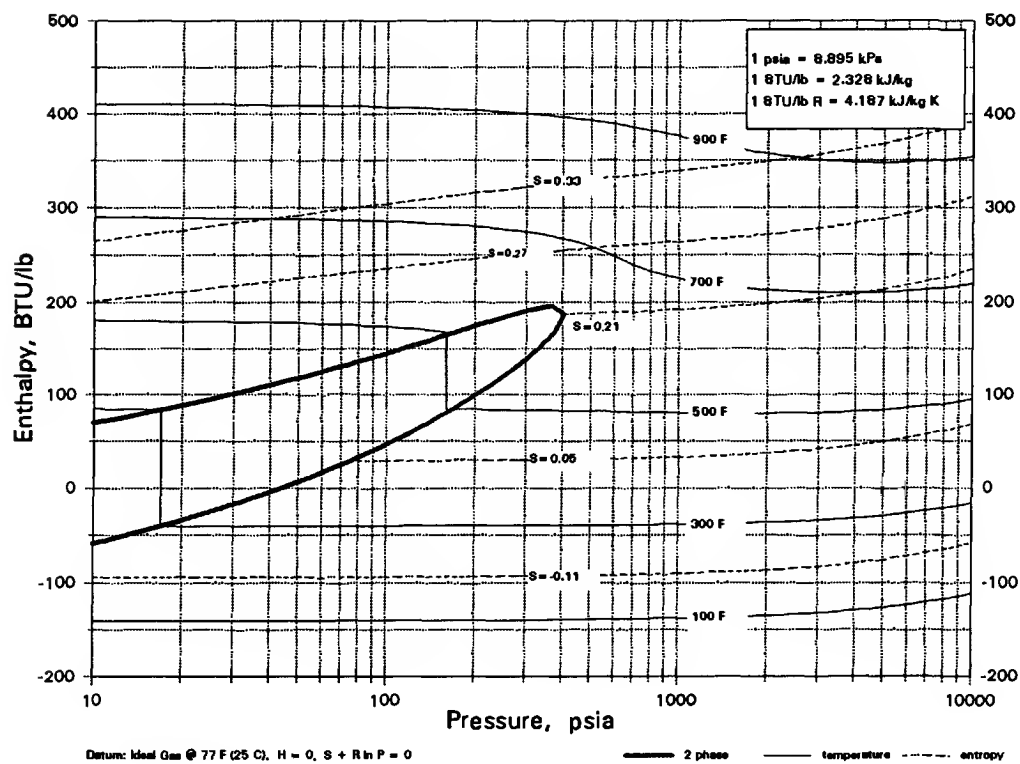
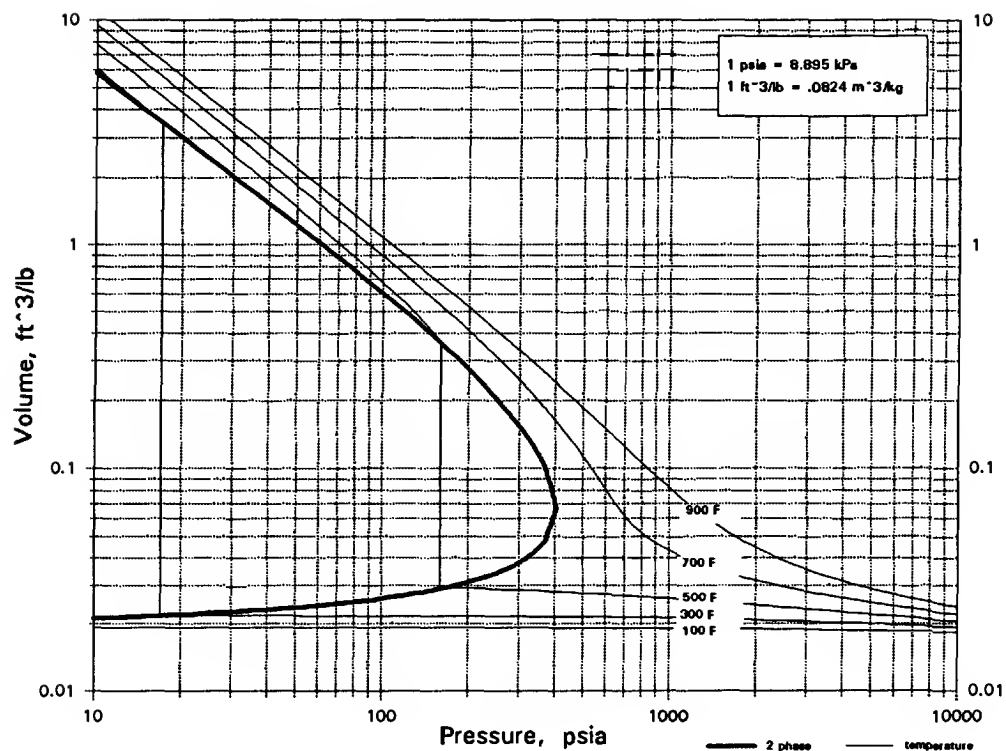
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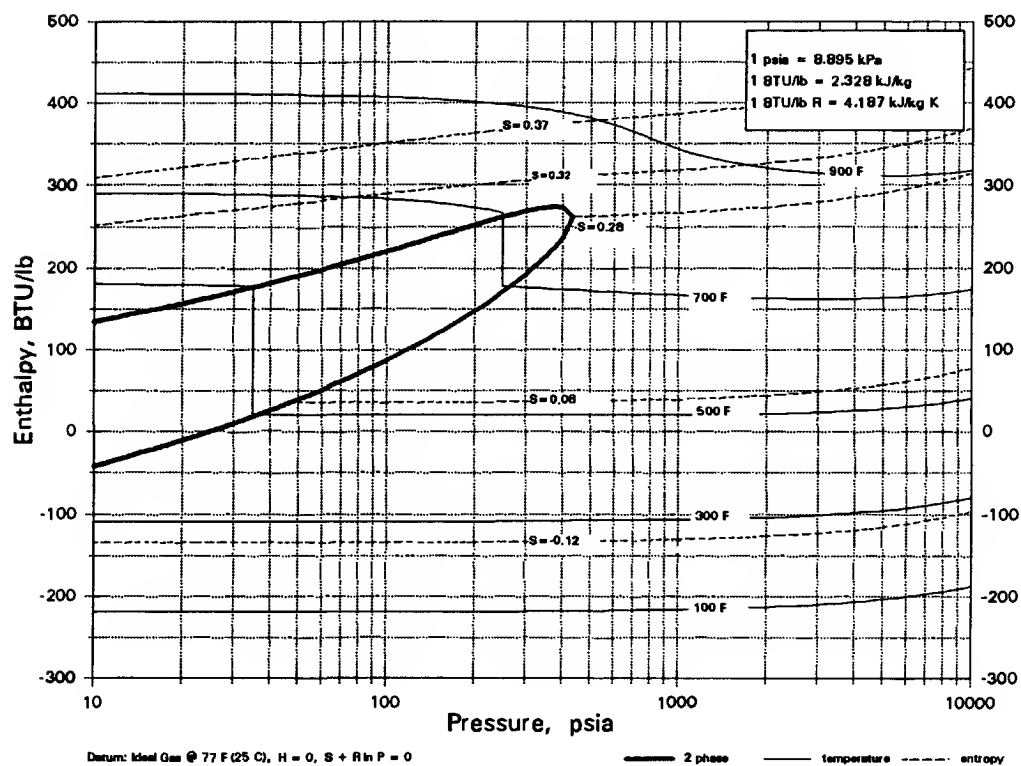
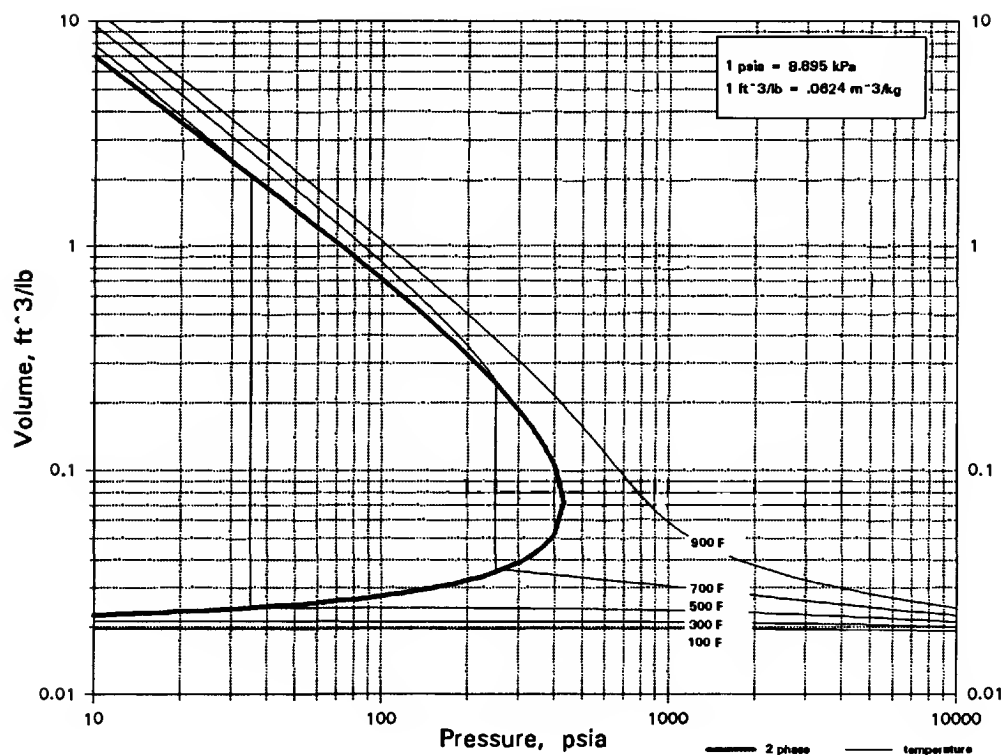
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n-PROPYL n-BUTYRATE



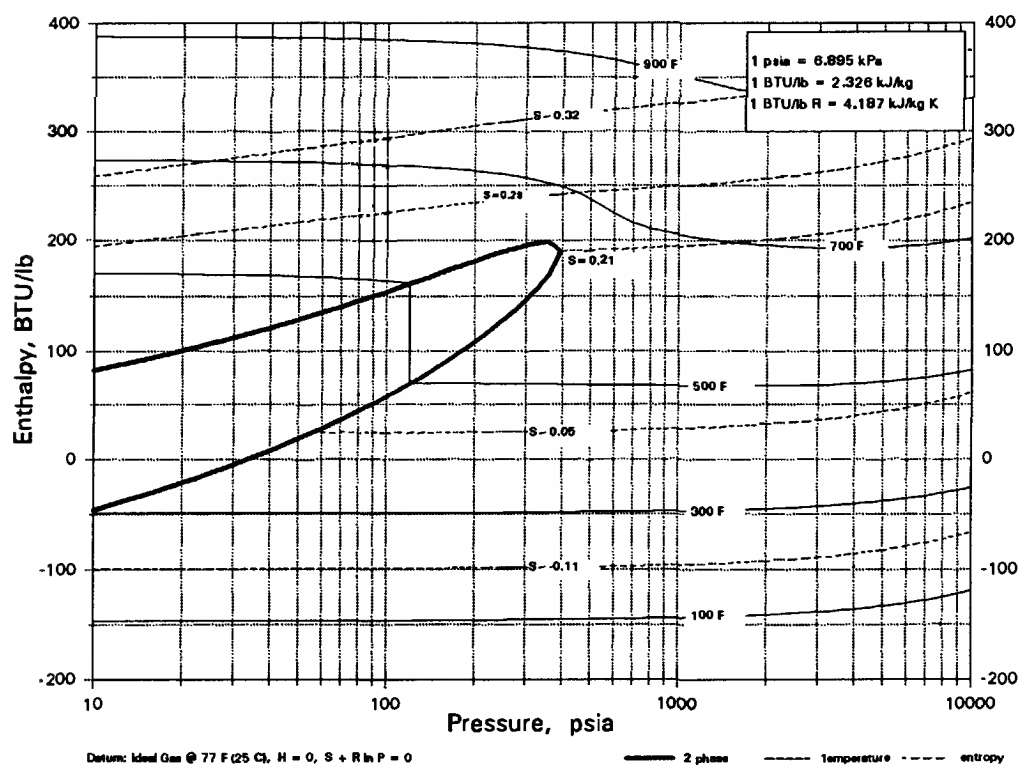
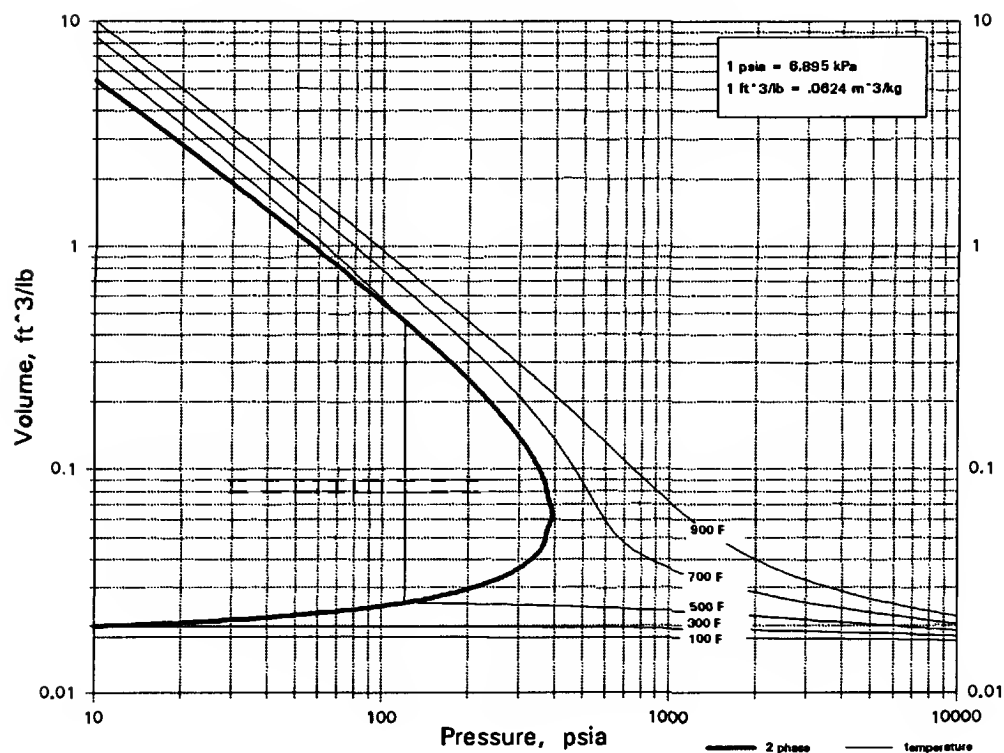
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n-HEPTANOIC ACID

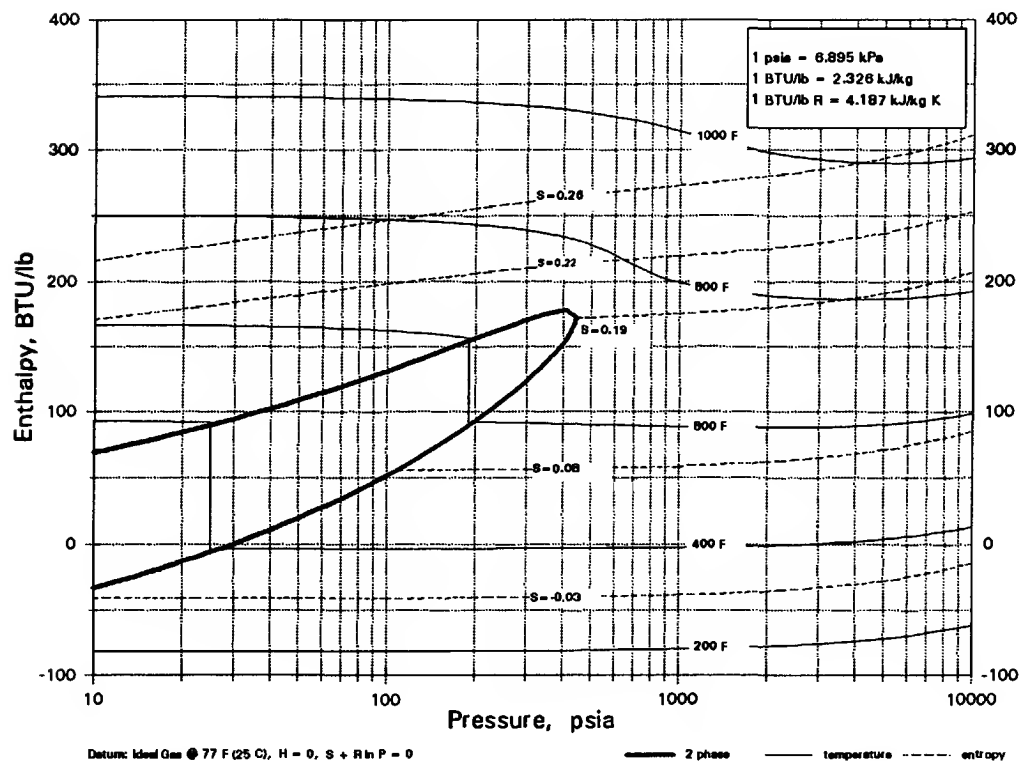
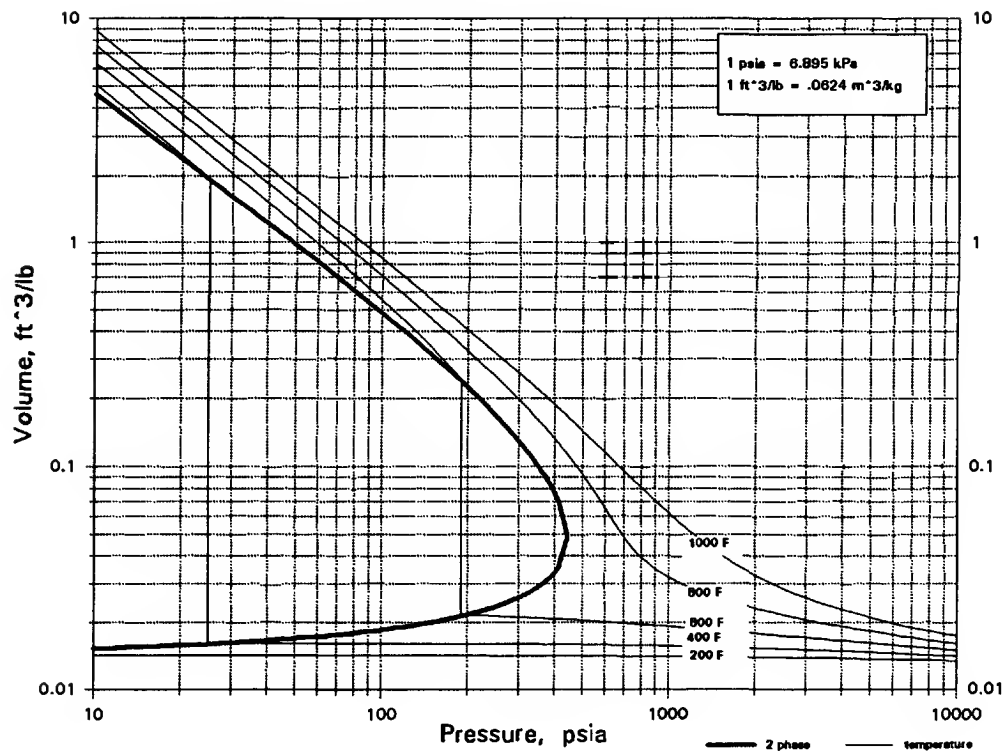


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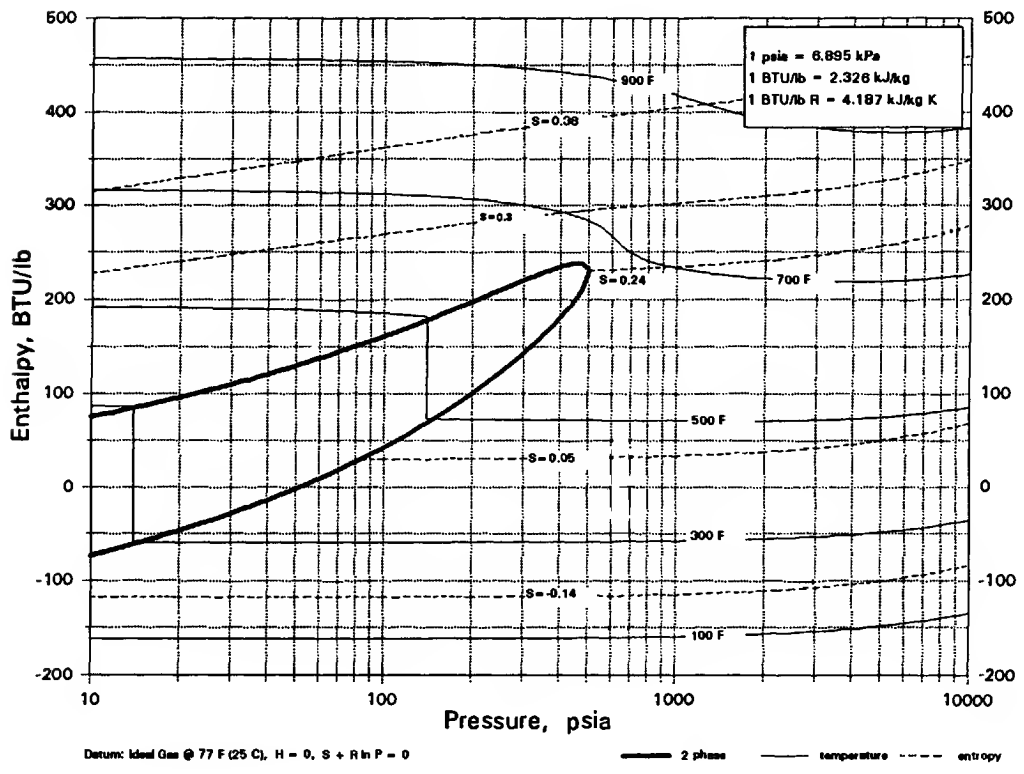
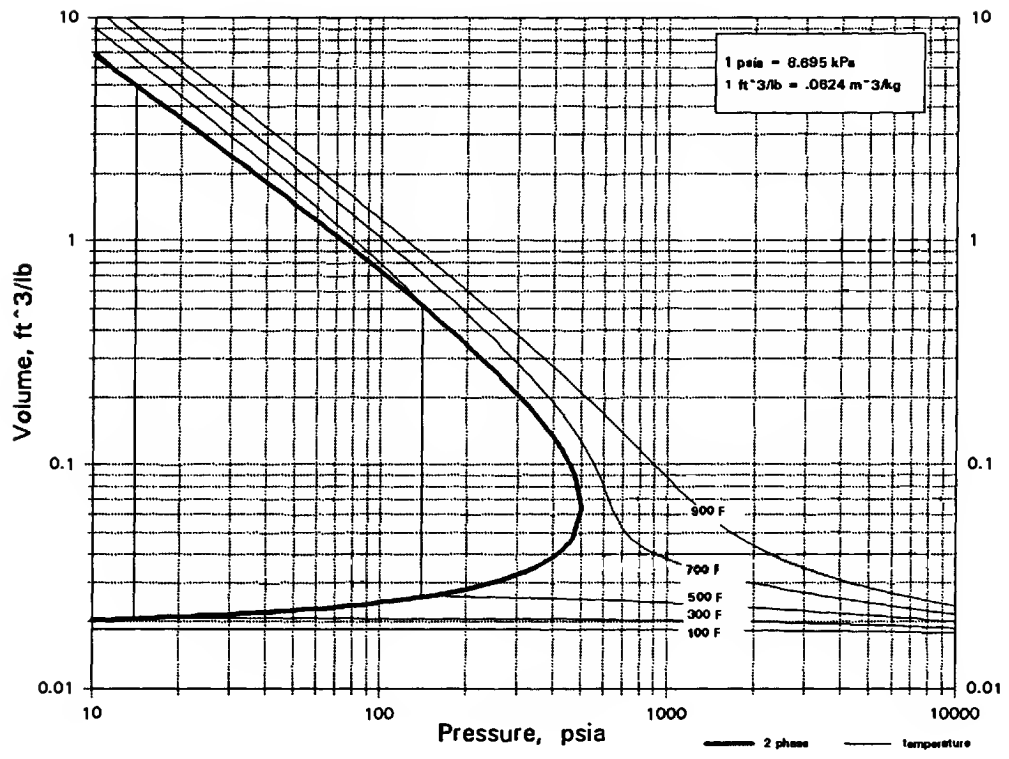
ETHYL-3-ETHOXYPROPIONATE



C7H15Br
1-BROMOHEPTANE

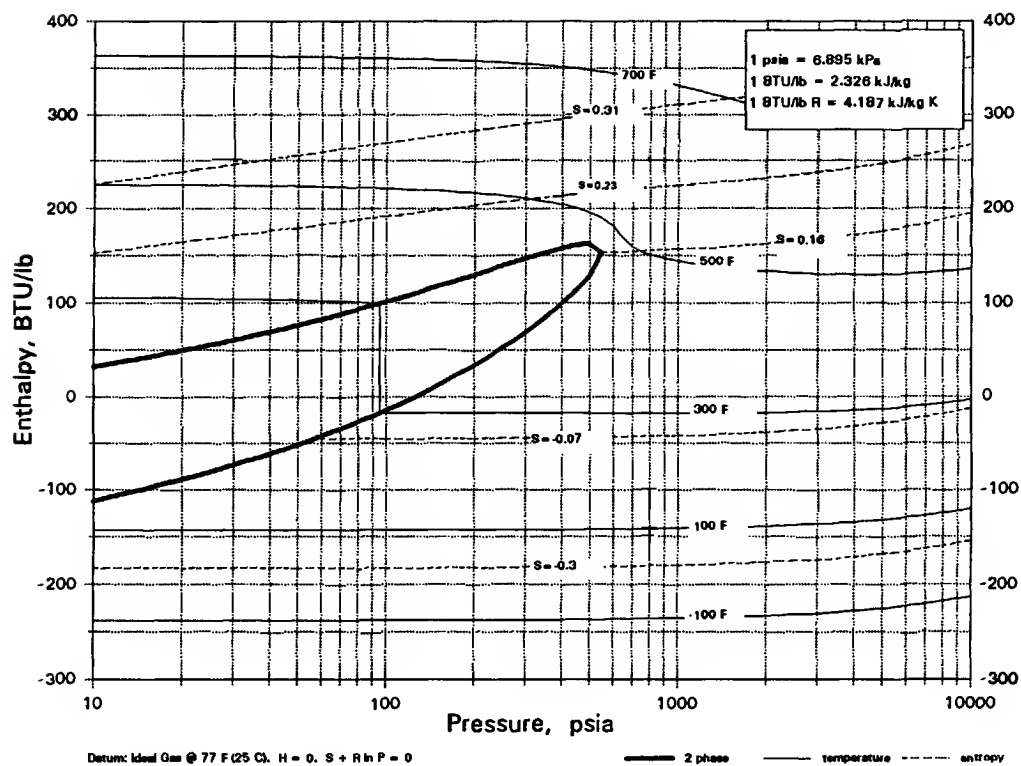
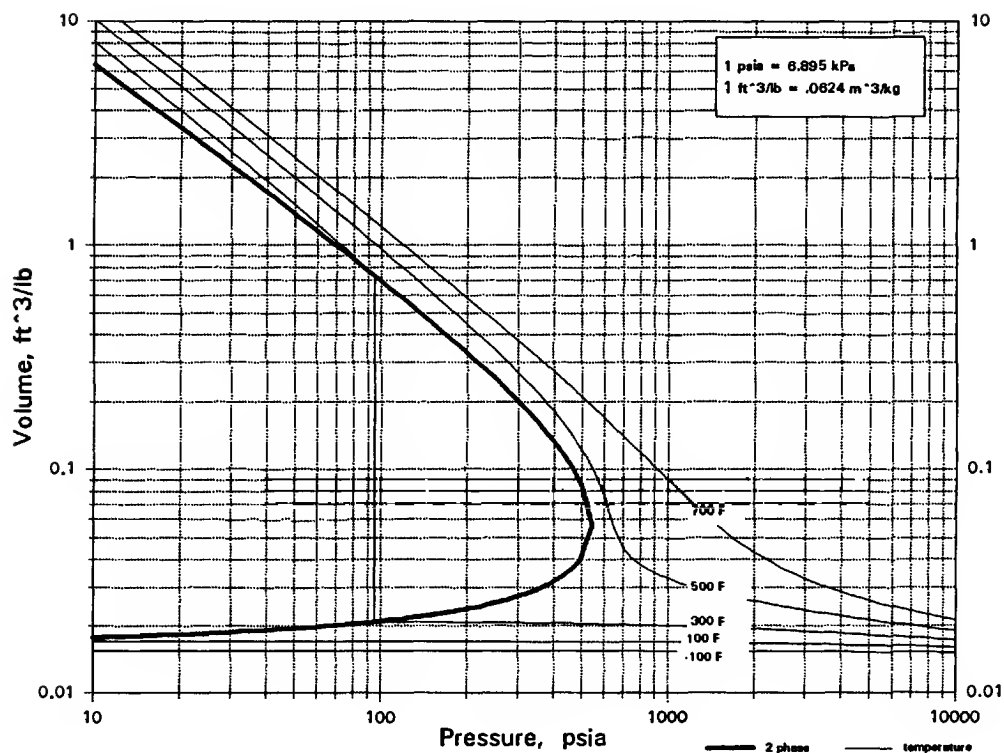


C7H15N
N-METHYLCYCLOHEXYLAMINE



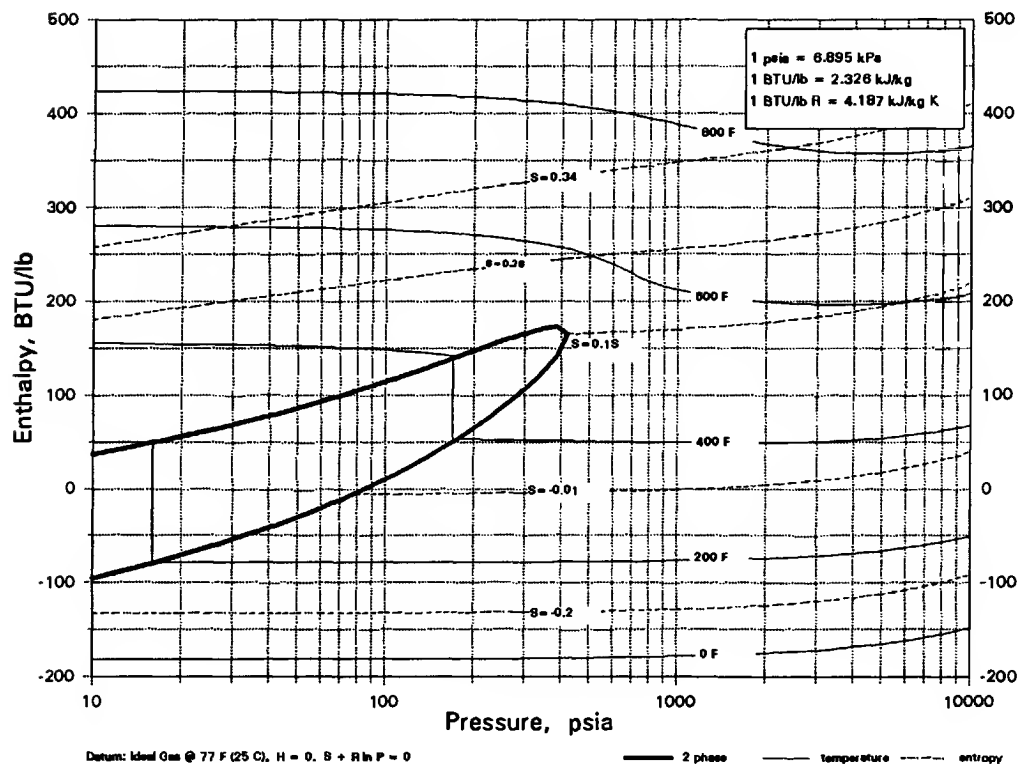
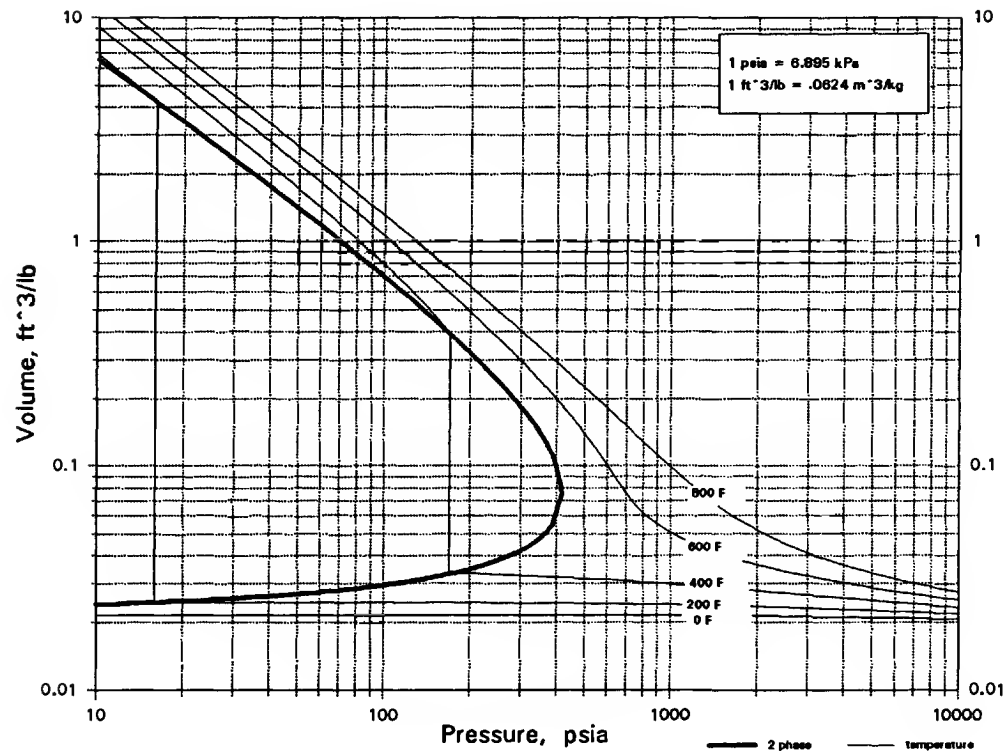
C7H16

2-2-DIMETHYLPENTANE



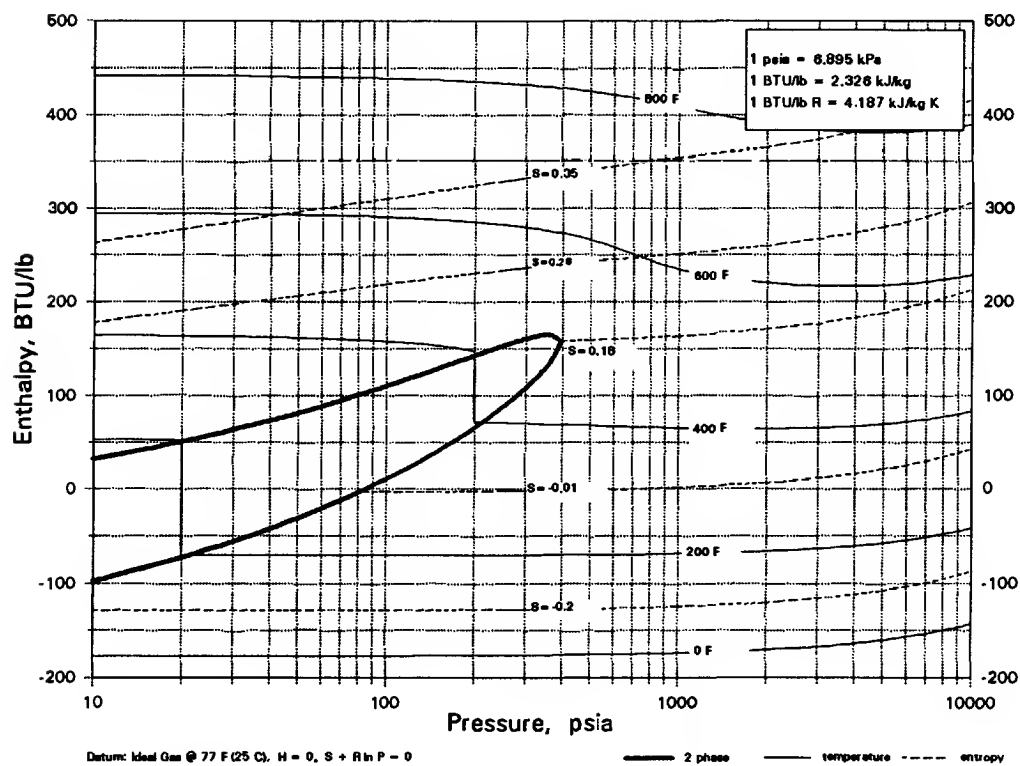
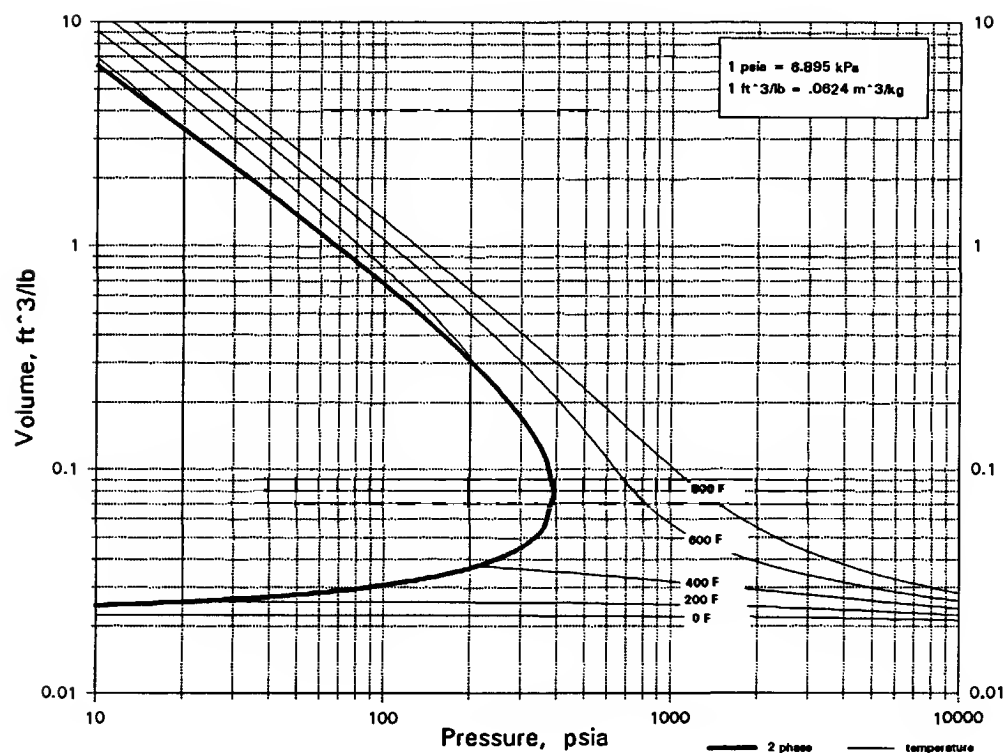
C7H16

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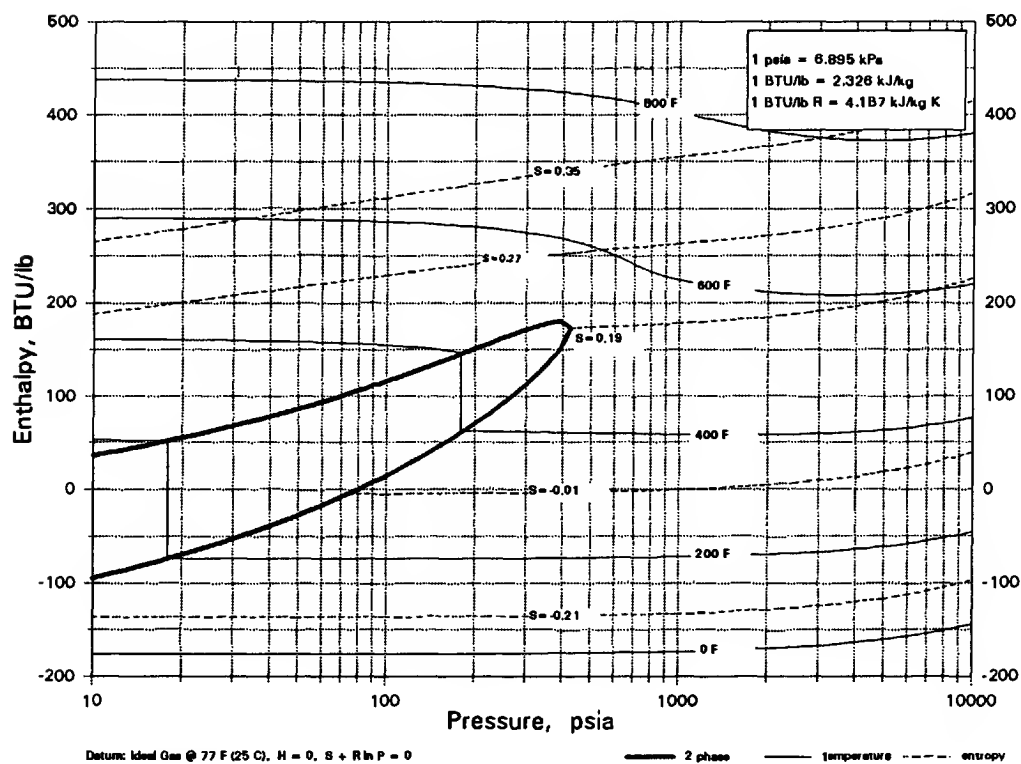
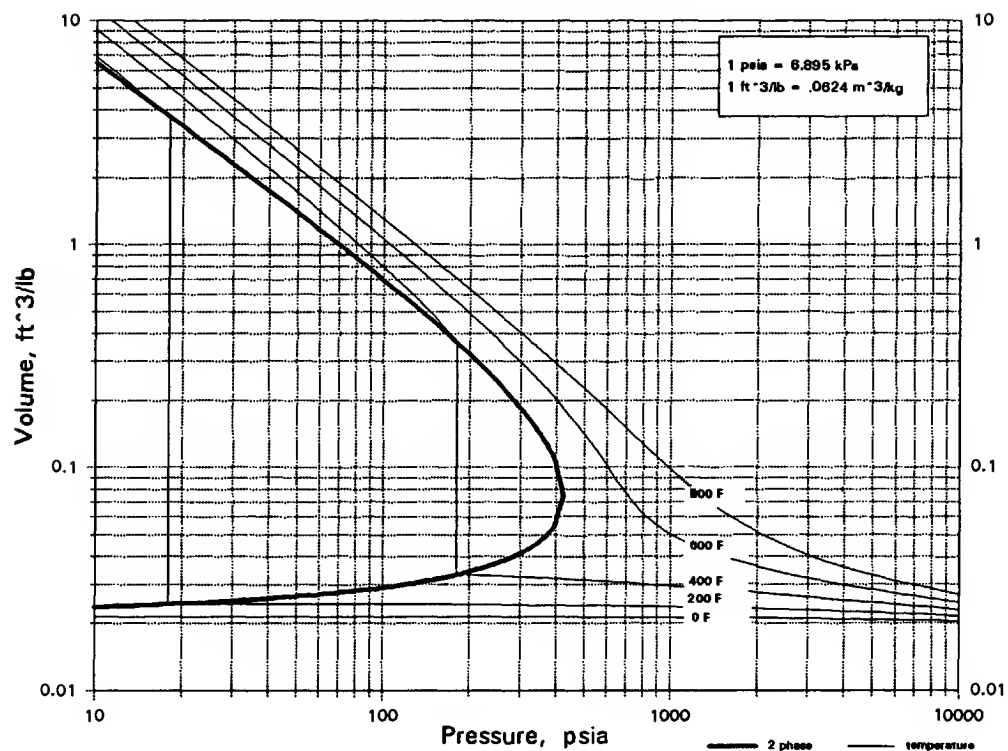
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2-4-DIMETHYLPENTANE



C7H16

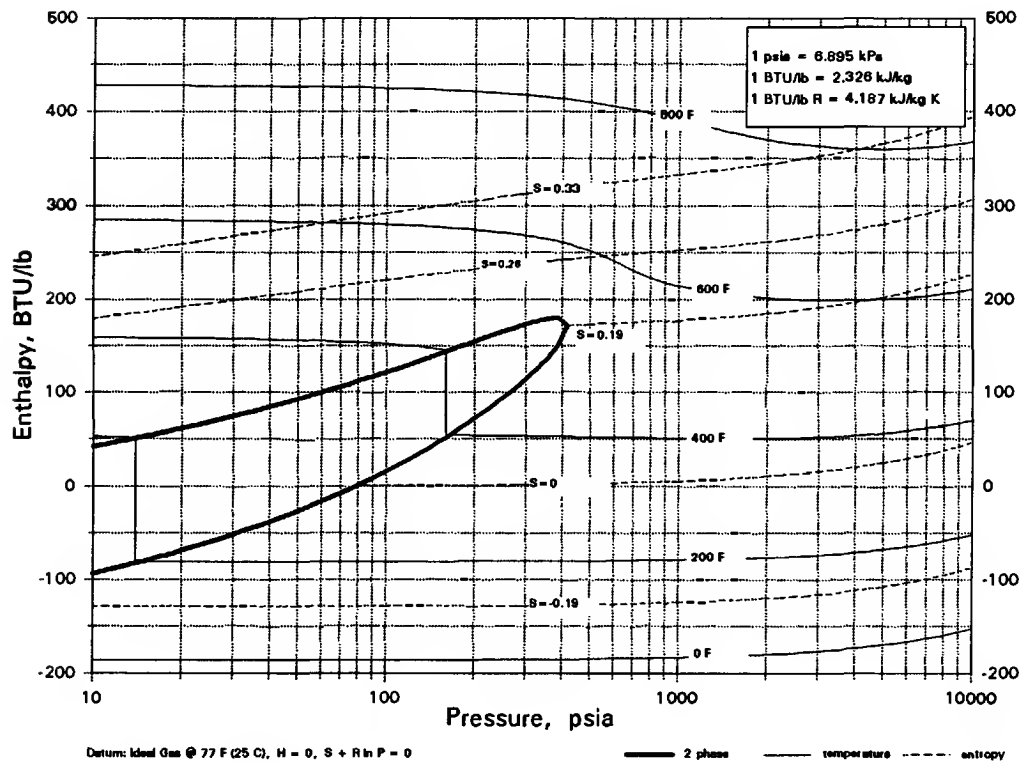
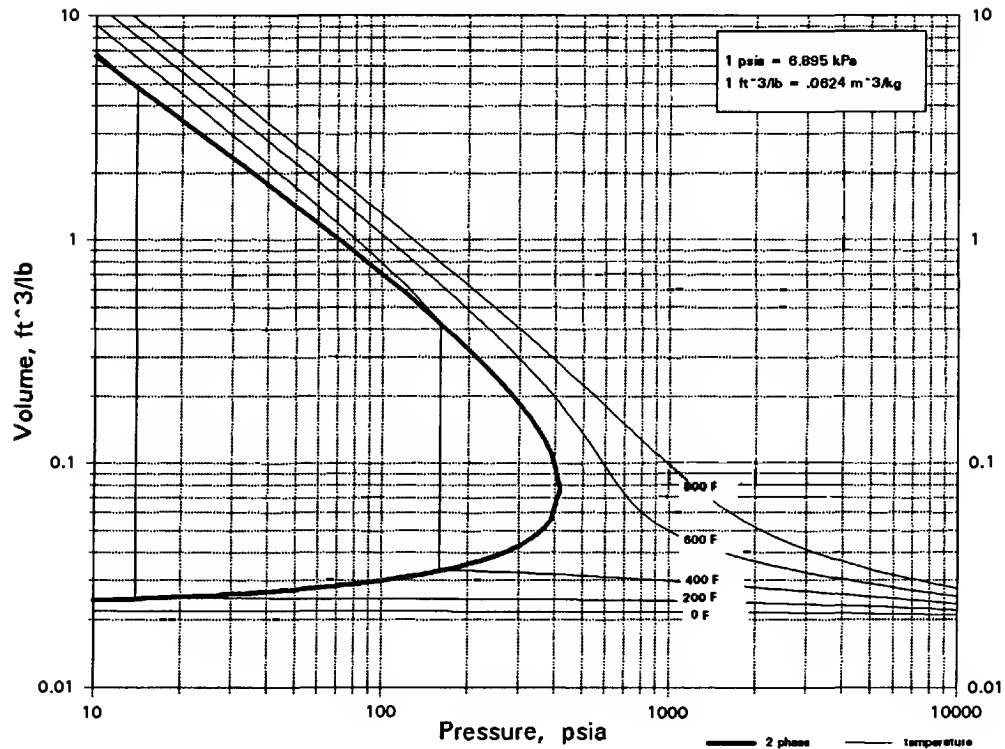
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Datum: Ideal Gas @ 77 F (25 C), H = 0, S + R ln P = 0

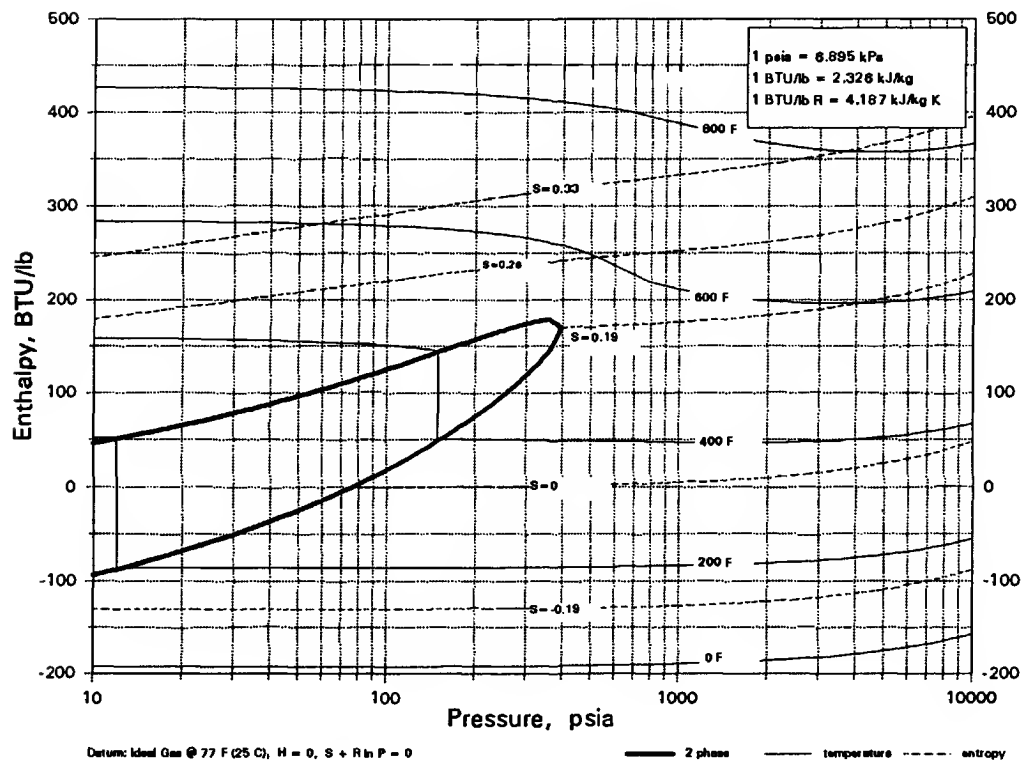
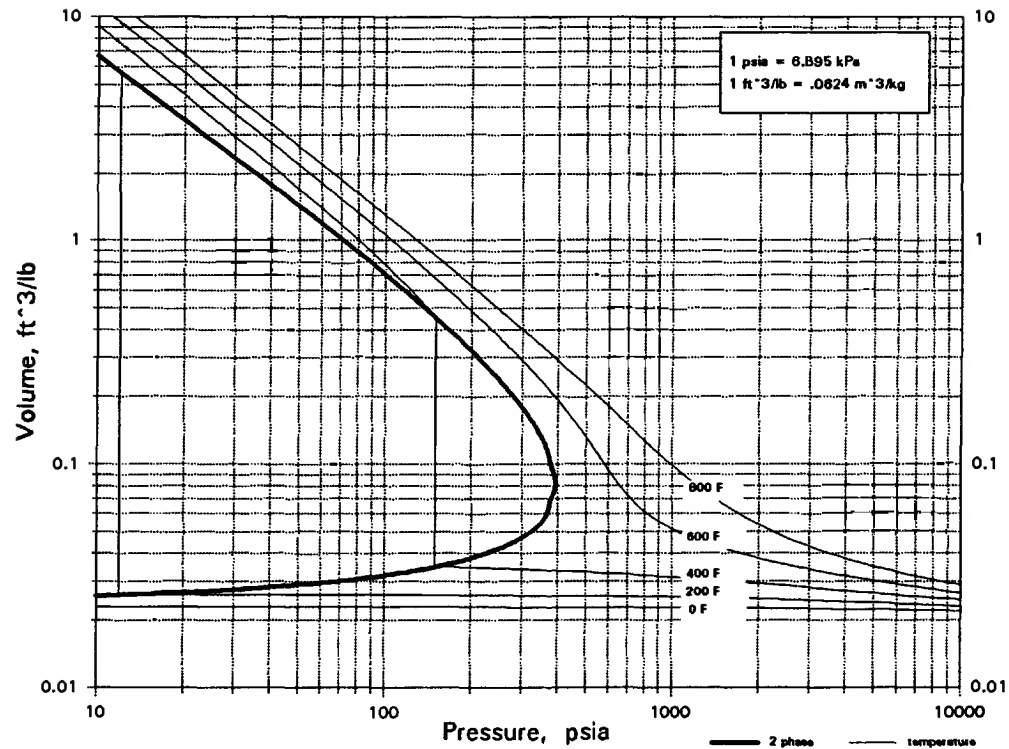
C7H16

3-ETHYLPENTANE



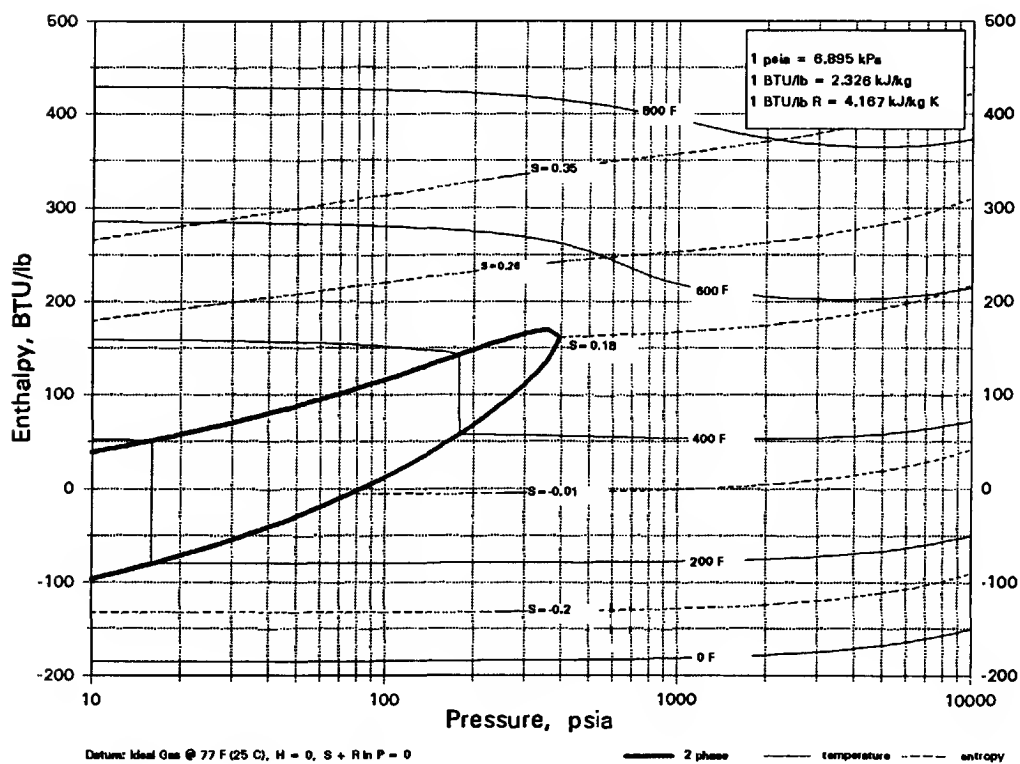
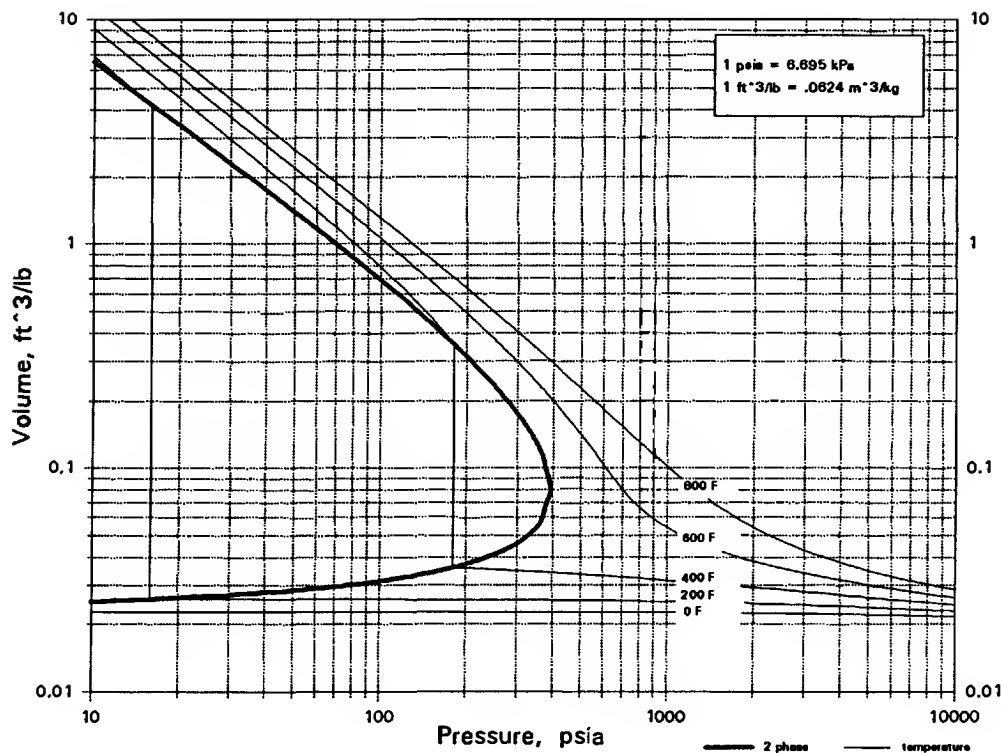
C7H16

n-HEPTANE



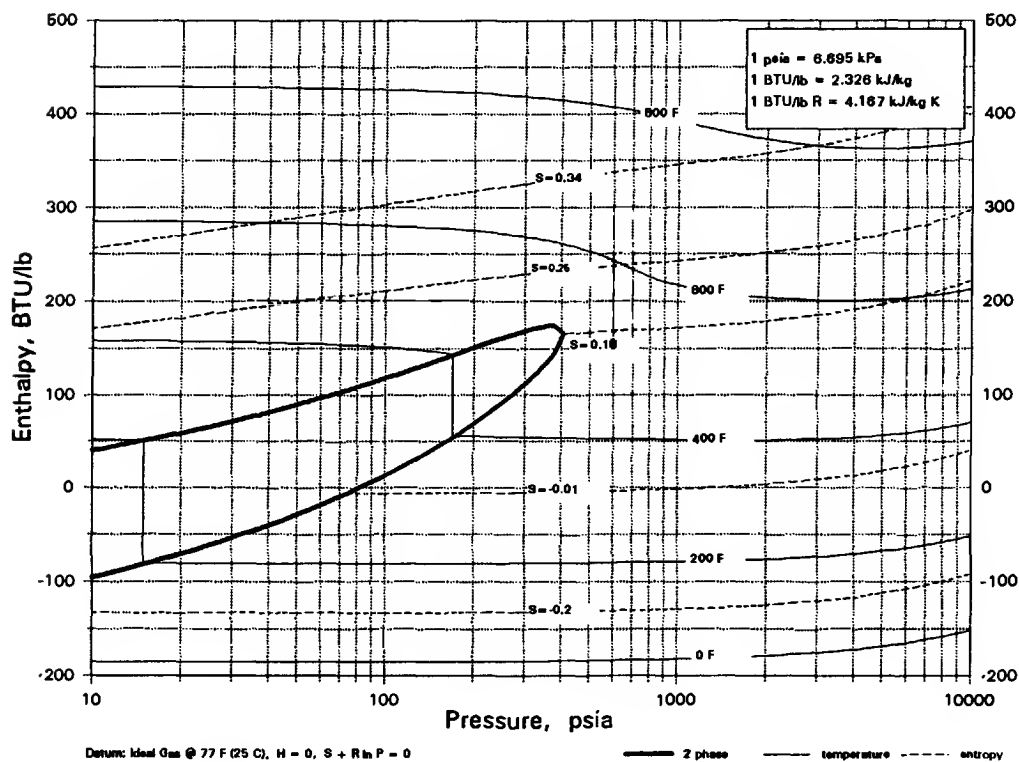
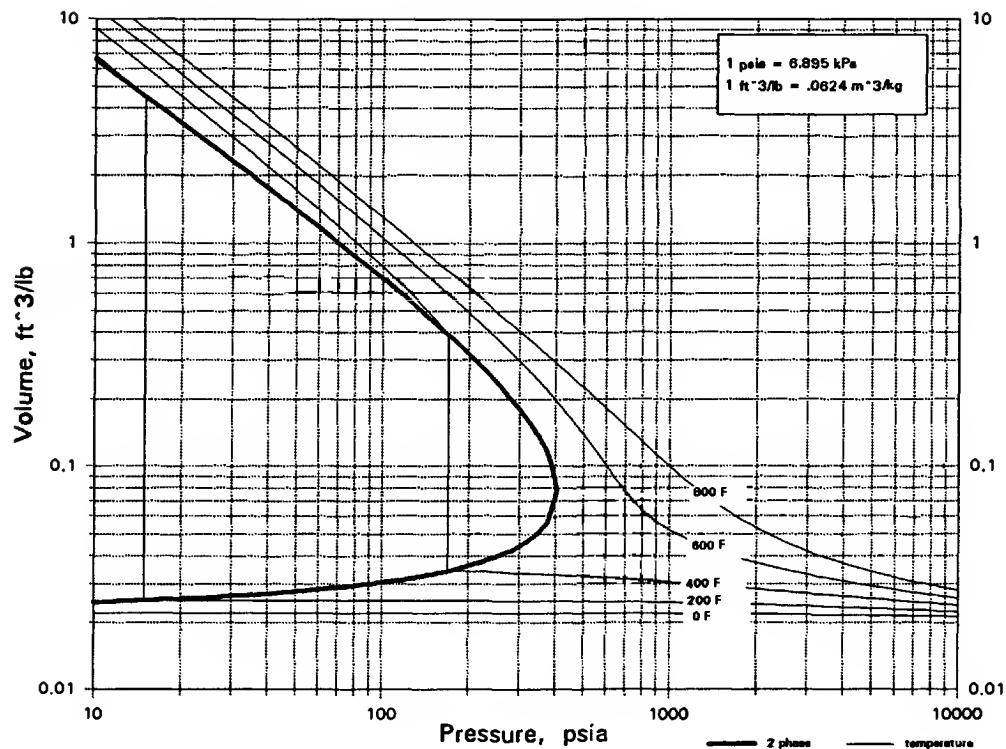
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2-METHYLHEXANE



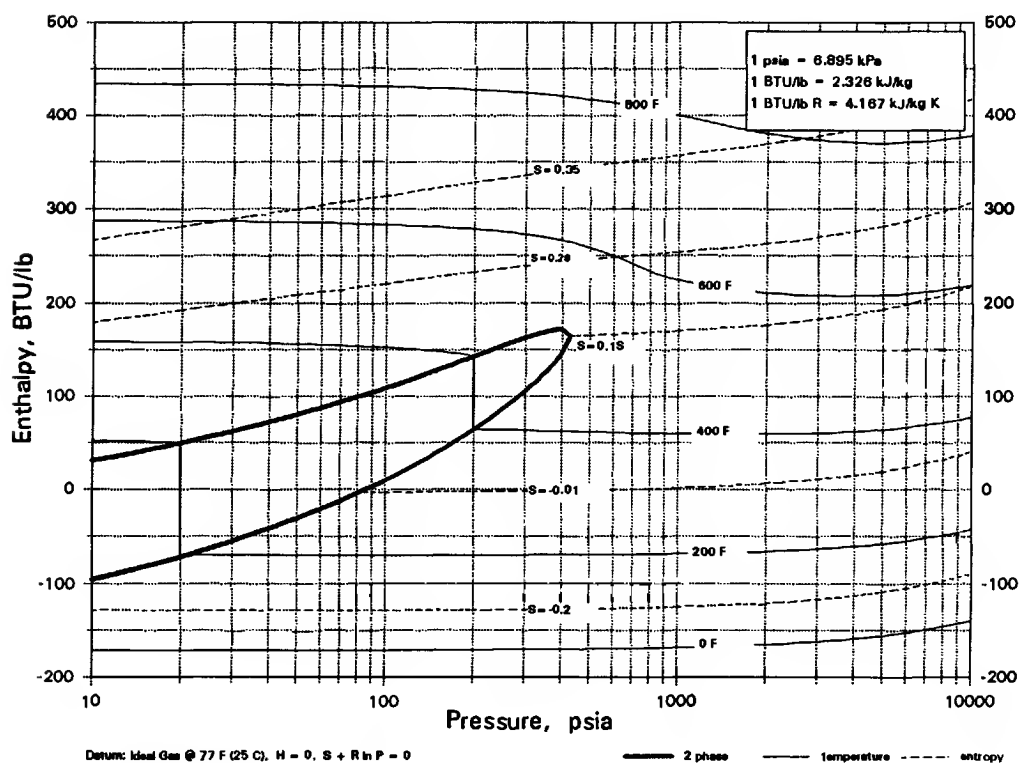
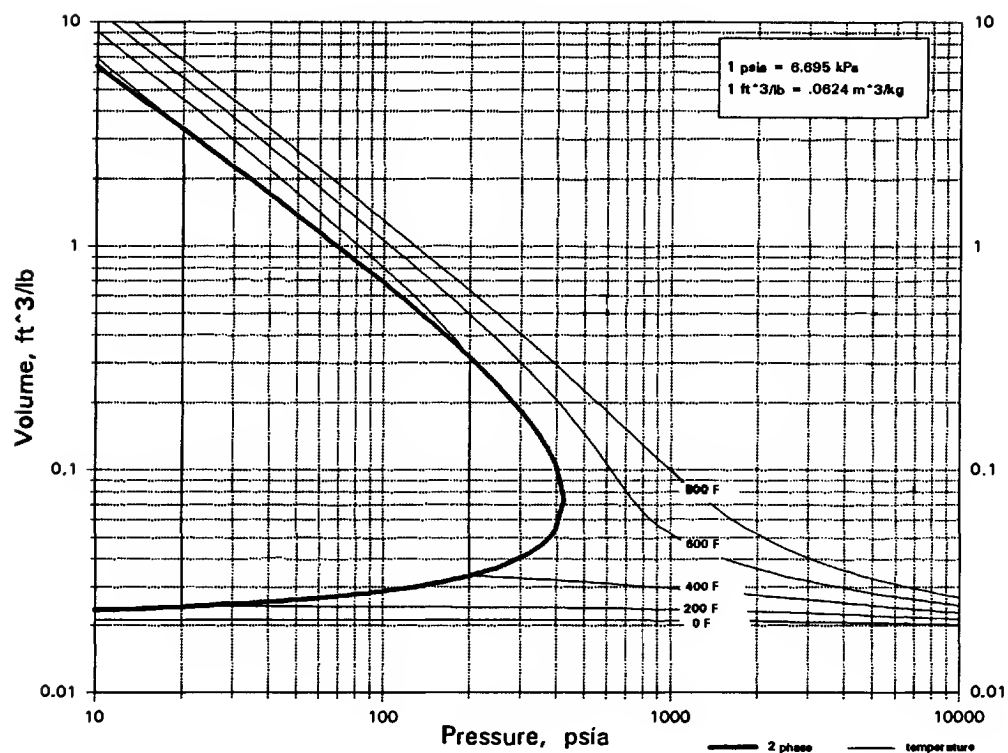
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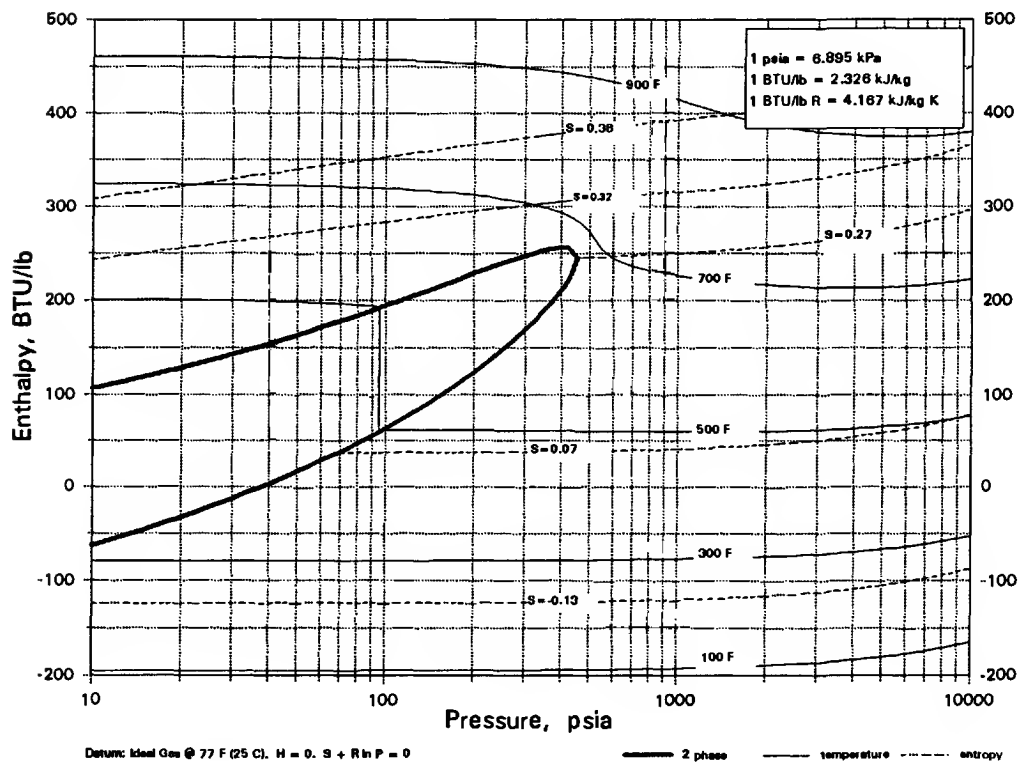
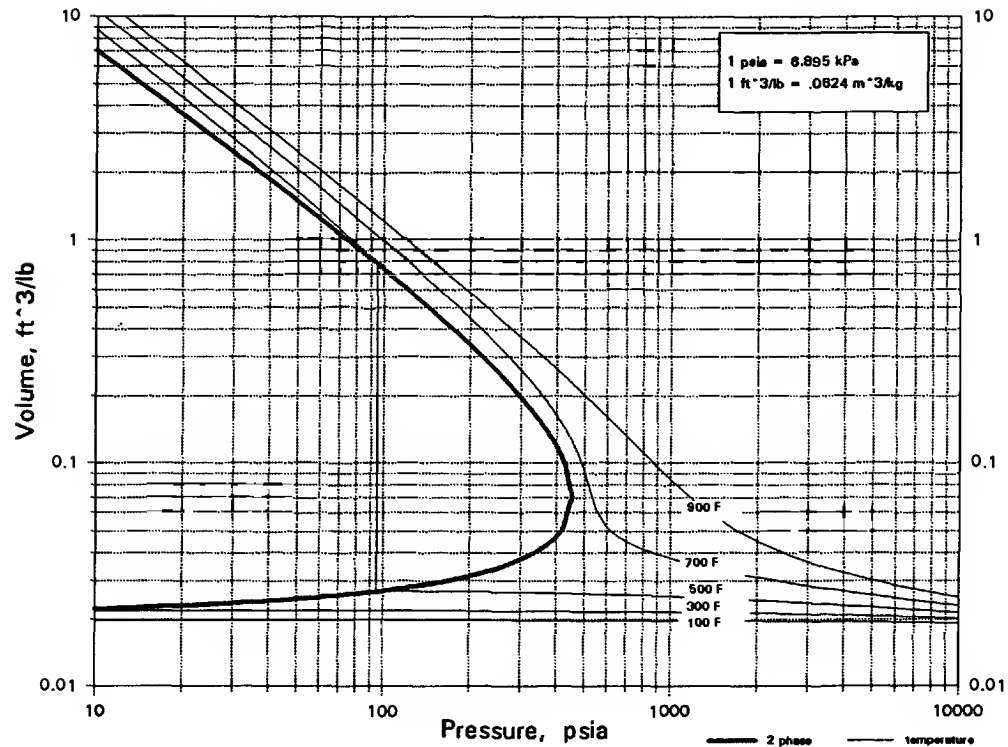
C7H16

2-2-3-TRIMETHYLBUTANE



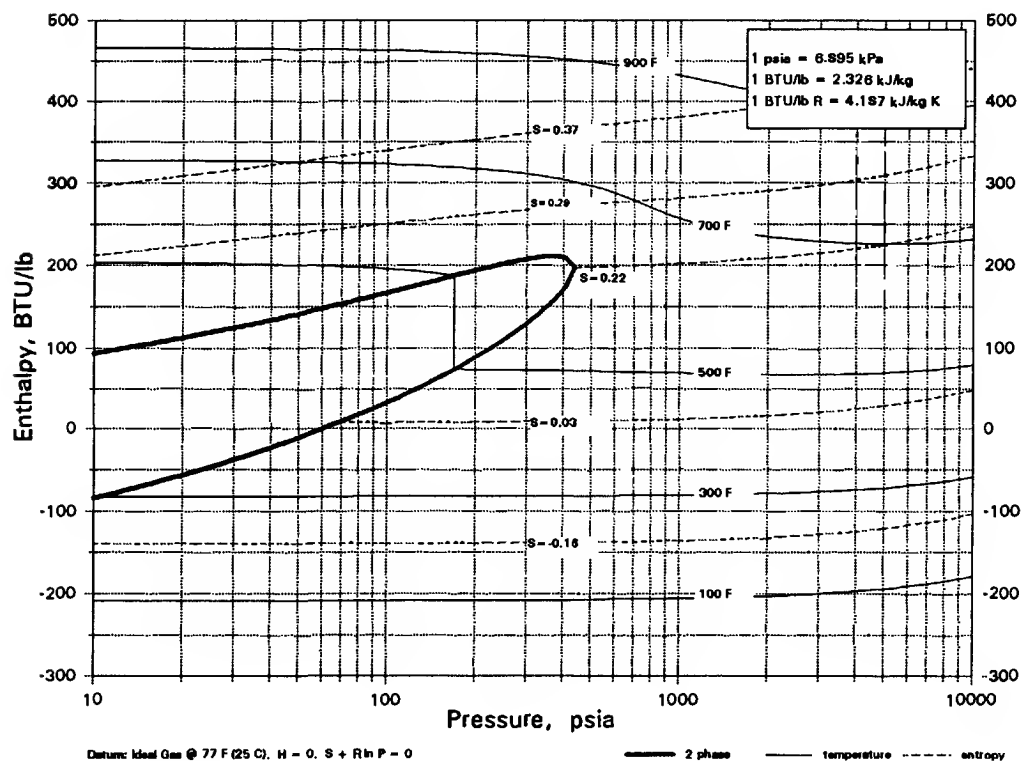
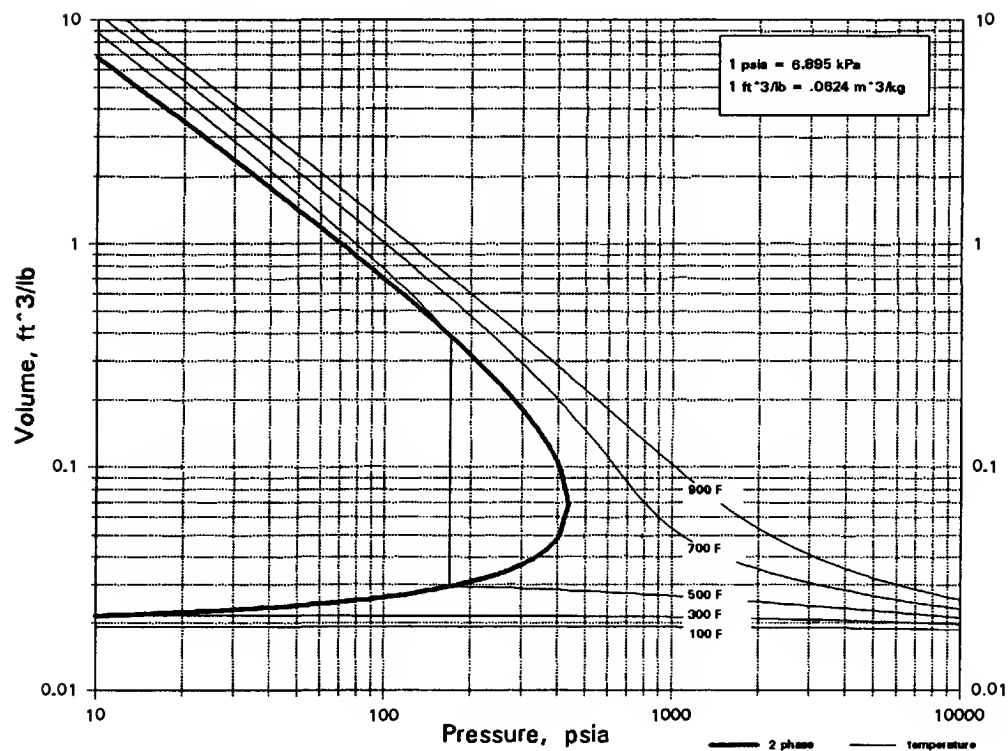
C7H16O

1-HEPTANOL



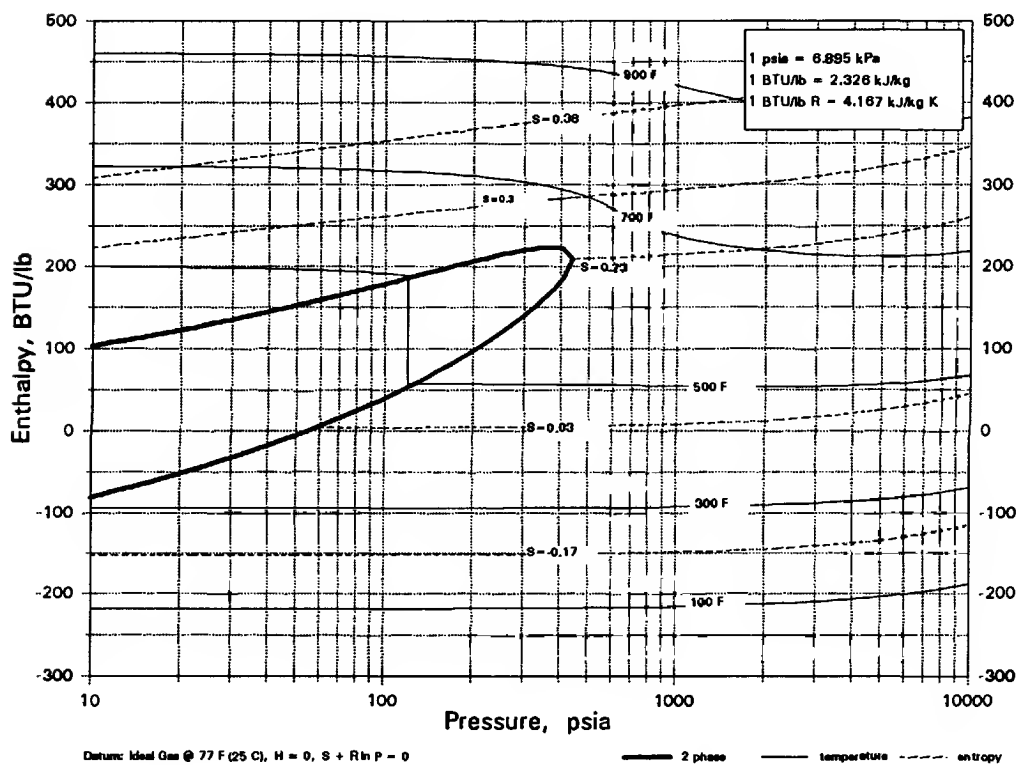
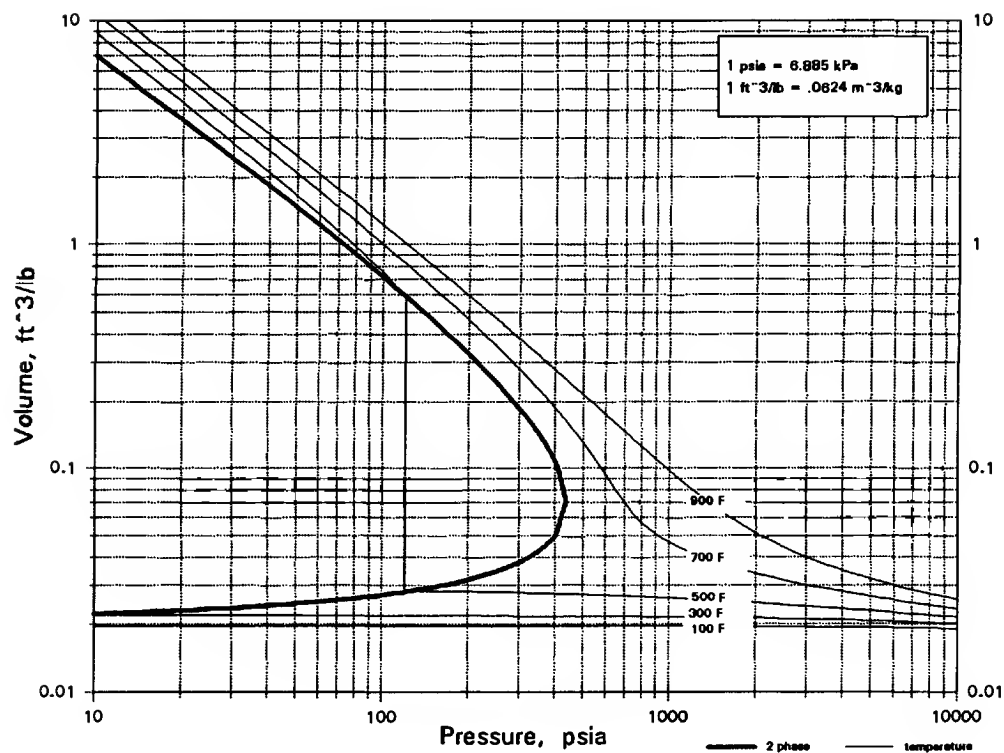
C7H16O

2-HEPTANOL



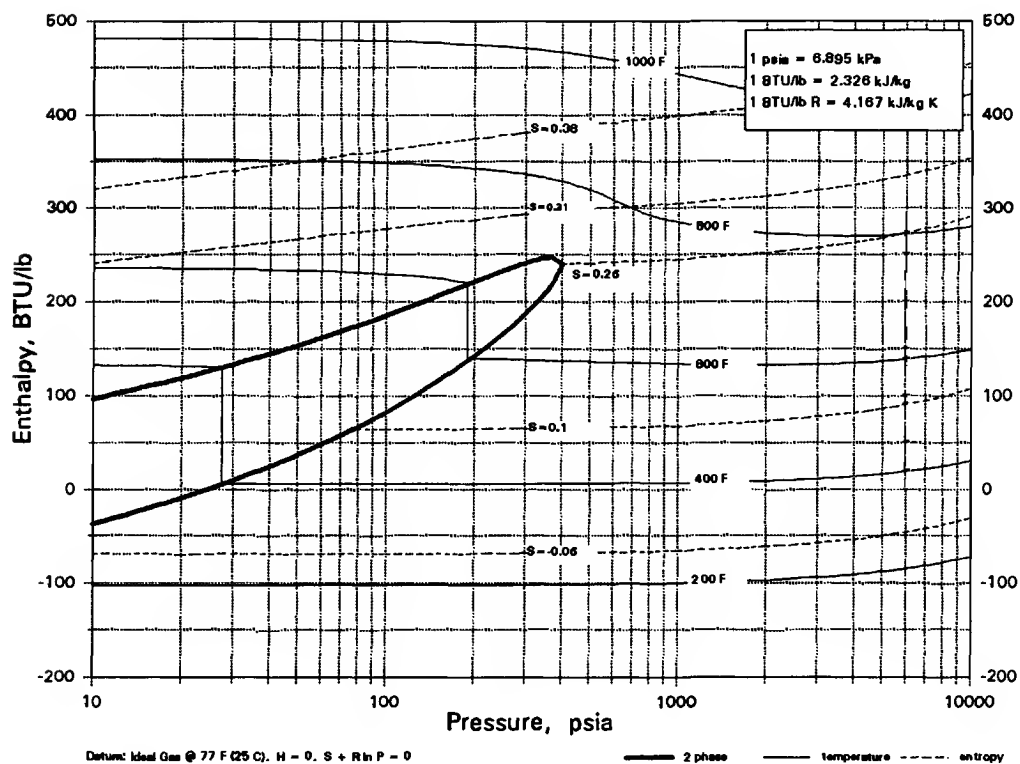
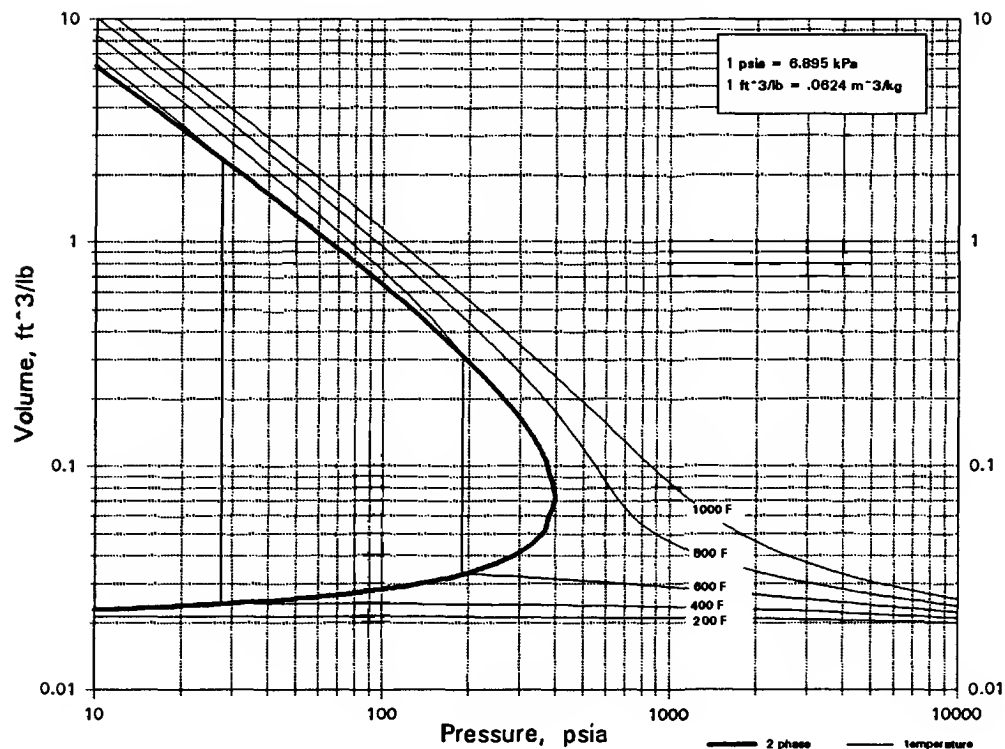
C7H16O

5-METHYL-1-HEXANOL



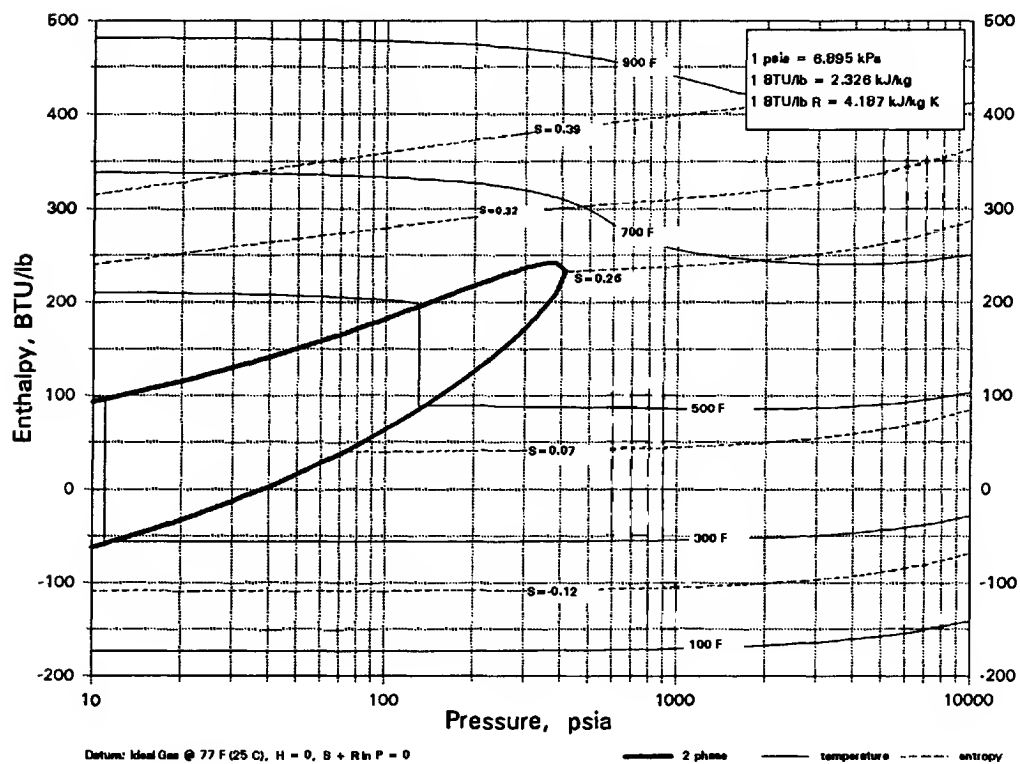
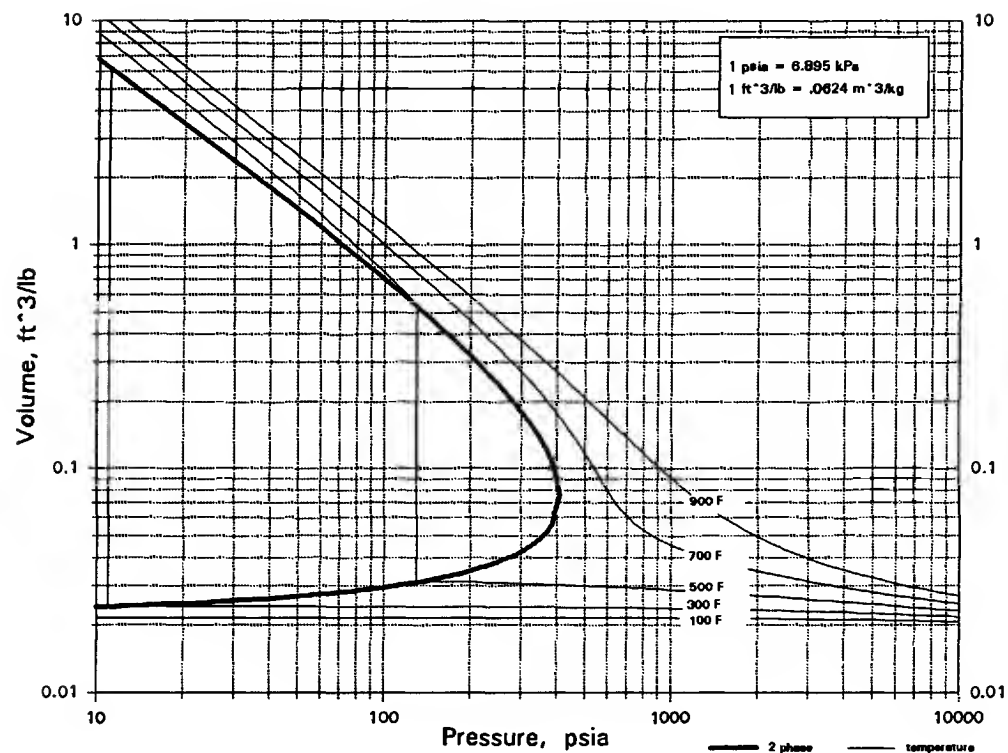
C7H16S

n-HEPTYL MERCAPTAN



C7H17N

1-AMINOHEPTANE



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Appendix A

Equations for Thermodynamic Properties

Enthalpy

$$H = H_{ref} + \int_{T_{ref}}^T C_p dT - \Delta H^{resid} \quad (1)$$

Entropy

$$S = S_{ref} + \int_{T_{ref}}^T \frac{C_p}{T} dT - R \ln\left(\frac{P}{P_{ref}}\right) - \Delta S^{resid} \quad (2)$$

Internal Energy

$$U = H - P V \quad (3)$$

Helmholtz Energy

$$A = U - T S \quad (4)$$

Gibbs Energy

$$G = H - T S \quad (5)$$

Parameters

$$C_p = \text{heat capacity of ideal gas} \quad (6)$$

$$H_{ref}, S_{ref} = \text{reference state for ideal gas} \quad (7)$$

$$T_{ref}, P_{ref} = \text{reference temperature, reference pressure} \quad (8)$$

$$\Delta H^{resid}, \Delta S^{resid} = \text{residual enthalpy, residual entropy} \quad (9)$$

Appendix B

Peng-Robinson Equation of State for Thermodynamic Properties

Equation of State

$$P = \frac{RT}{V - b} - \frac{a}{V(V + b) + b(V - b)} \quad (1)$$

Volume

$$V^3 + (b - \frac{RT}{P})V^2 + (\frac{a}{P} - 3b^2 - \frac{RT}{P}2b)V + (b^3 + \frac{RT}{P}b^2 - \frac{ab}{P}) = 0 \quad (2)$$

Compressibility Factor

$$Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \quad (3)$$

Fugacity Coefficient

$$\ln \phi = Z - 1 - \ln(Z - B) - \frac{A}{2\sqrt{2}B} \ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \quad (4)$$

Residual Enthalpy

$$\frac{\Delta H^{resid}}{RT} = 1 - Z + \frac{A}{2\sqrt{2}B} \left(1 + \frac{D}{a}\right) \ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \quad (5)$$

Residual Entropy

$$\frac{\Delta S^{resid}}{R} = -\ln(Z - B) + \frac{AD}{2\sqrt{2}Ba} \ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \quad (6)$$

Parameters

$$a = a_c \alpha \quad (7)$$

$$a_c = 0.45724R^2T_c^2/P_c \quad (8)$$

$$b = 0.07780RT_c/P_c \quad (9)$$

$$\alpha = [1 + m(1 - T_r^{1/2})]^2 \quad (10)$$

$$m = 0.37464 + 1.54226\Omega - 0.26992\Omega^2 \text{ (original PR)} \quad (11)$$

$$m = \text{see Stryjek , Vera (modified PR)} \quad (12)$$

$$A = aP/R^2T^2 = 0.45724\alpha P_r/T_r^2 = 0.45724 \frac{(P/P_c)}{(T/T_c)^2} \alpha \quad (13)$$

$$B = bP/RT = 0.07780P_r/T_r = 0.07780 \frac{(P/P_c)}{(T/T_c)} \quad (14)$$

$$D = -T \frac{da}{dT} = ma\sqrt{T_r/\alpha} \quad (15)$$

Appendix C

Examples for Thermodynamic Diagrams

Example 1 - Vessel Pressure

A vessel containing gaseous 1-pentene (C₅H₁₀) at 260 psia and 300 F is exposed to a fire in the process area. The temperature in the vessel is 700 F when the fire is extinguished. Estimate the final pressure in the vessel.

Since the vessel size does not change appreciably, this situation may be approximated by a constant volume process. Using the thermodynamic diagram, the initial volume is about 0.3 ft³/lb. At this same volume and final temperature, the pressure is:

$$\underline{P_{\text{final}} = 520 \text{ psia}}$$

Example 2 - Reactor Size

A batch reactor is to contain 2,000 lb of 1-pentene (C₅H₁₀) at 400 psia and 500 F. Estimate the reactor size.

Using the thermodynamic diagram, the volume is about 0.3 ft³/lb at these conditions. Substitution of this into the equation below for the reactor size provides:

$$\underline{\text{Reactor Size} = (2,000 \text{ lb}) (0.3 \text{ ft}^3/\text{lb}) = 600 \text{ ft}^3}$$

Example 3 - Process Vessel Size

A process vessel is to contain 500 lb of 1-pentene (C₅H₁₀) at 100 psia and 500 F. Estimate the process vessel size.

Using the thermodynamic diagram, the volume is about 1 ft³/lb at these conditions. Substitution of this into the equation below for the process vessel size provides:

$$\underline{\text{Vessel Size} = (500 \text{ lb}) (1 \text{ ft}^3/\text{lb}) = 500 \text{ ft}^3}$$

Example 4 - Heat Exchanger Duty

1-Pentene (C₅H₁₀, 30,000 lb/hr) at 1,000 psia and 100 F is heated to 500 F and then fed to a plug-flow reactor. Estimate the heat exchanger duty necessary to accomplish the heating.

Substitution of mass flow and enthalpies from the thermodynamic diagram into the equation below provides:

$$\begin{aligned} \underline{\text{Heat Exchanger Duty} = \text{mass flow} (H_2 - H_1) = (30,000 \text{ lb/hr})(145 - (-145)) \text{ BTU/lb}} \\ = \underline{8.7 \text{ million BTU/hr}} \end{aligned}$$

Example 5 - Compression

1-Pentene (C₅H₁₀, 20,000 lb/hr) at 50 psia and 300 F is compressed to 6,500 psia. Estimate the change in enthalpy for the compression assuming adiabatic and reversible conditions (constant entropy).

Substitution of mass flow and enthalpies from the thermodynamic diagram into the equation below provides:

$$\begin{aligned}\text{Enthalpy Change} &= \text{mass flow } (H_2 - H_1) = (20,000 \text{ lb/hr})(200 - 100) \text{ BTU/lb} \\ &= \underline{2.0 \text{ million BTU/hr}}\end{aligned}$$

This change in enthalpy represents energy that is required to accomplish the compression under adiabatic and reversible conditions. Under operating conditions, the actual energy that is required for the compression will be somewhat more depending on the efficiency.

Example 6 - Expansion

1-Pentene (C₅H₁₀, 30,000 lb/hr) at 2,000 psia and 700 F is expanded to 10 psia. Estimate the change in enthalpy for the expansion assuming adiabatic and reversible conditions (constant entropy).

Substitution of mass flow and enthalpies from the thermodynamic diagram into the equation below provides:

$$\begin{aligned}\text{Enthalpy Change} &= \text{mass flow } (H_2 - H_1) = (30,000 \text{ lb/hr})(145 - 275) \text{ BTU/lb} \\ &= \underline{- 3.9 \text{ million BTU/hr}}\end{aligned}$$

This change in enthalpy represents energy that is available from the expansion under adiabatic and reversible conditions. Under operating conditions, the actual energy that is available for the expansion will be somewhat less depending on the efficiency.

Appendix D

CRITICAL CONSTANTS AND ACENTRIC FACTOR FOR C₆ TO C₇ COMPOUNDS

Carl L. Yaws
Lamar University, Beaumont, Texas

NO	FORMULA	NAME	MW g/mol	T _F K	T _B K	T _C K	P _C bar	V _C cm ³ /mol	ρ _C g/cm ³	Z _C	ω
1	C5Cl6	HEXACHLOROCYCLOPENTADIENE	272.771	284.49	512.15	746.00	30.10	526.0	0.5186	0.255	0.369
2	C5H4O2	FURFURAL	96.086	236.65	434.85	657.00	55.12	252.0	0.3813	0.254	0.444
3	C5H5N	PYRIDINE	79.101	231.53	388.41	619.95	56.34	254.0	0.3114	0.278	0.239
4	C5H6	CYCLOPENTADIENE	66.103	188.15	314.65	507.00	51.50	225.0	0.2938	0.275	0.212
5	C5H6	2-METHYL-1-BUTENE-3-YNE	66.103	160.15	305.40	492.00	43.80	248.0	0.2665	0.266	0.137
6	C5H6	1-PENTENE-3-YNE	66.103	---	332.40	520.00	44.00	256.0	0.2582	0.261	0.252
7	C5H6	1-PENTENE-4-YNE	66.103	---	315.65	503.00	44.00	256.0	0.2582	0.269	0.179
8	C5H6N2	GLUTARONITRILE	94.116	244.21	559.15	782.00	31.50	352.0	0.2674	0.171	0.603
9	C5H6O2	FURFURYL ALCOHOL	98.101	258.52	443.15	632.00	53.50	263.0	0.3730	0.268	0.736
10	C5H6O3	GLUTARIC ANHYDRIDE	114.101	328.00	562.69	838.00	58.00	275.0	0.4149	0.229	0.537
11	C5H6O4	CITRACONIC ACID	130.100	356.15	607.00	829.00	42.40	340.0	0.3826	0.209	0.927
12	C5H6O4	ITACONIC ACID	130.100	438.75	601.00	821.00	42.40	340.0	0.3826	0.211	0.925
13	C5H7N	N-METHYLPYRROLE	81.117	216.91	385.89	610.00	47.70	283.0	0.2866	0.266	0.213
14	C5H7NO2	ETHYL CYANOACETATE	113.116	250.65	479.15	679.00	33.40	358.0	0.3160	0.212	0.573
15	C5H8	CYCLOPENTENE	68.118	138.13	317.38	507.00	47.90	240.0	0.2838	0.273	0.195
16	C5H8	ISOPRENE	68.118	127.27	307.21	484.00	38.50	276.0	0.2468	0.264	0.158
17	C5H8	3-METHYL-1-2-BUTADIENE	68.118	159.53	314.00	490.00	38.30	291.0	0.2341	0.274	0.187
18	C5H8	1-2-PENTADIENE	68.118	135.89	318.01	500.00	38.00	276.0	0.2468	0.252	0.154
19	C5H8	cis-1-3-PENTADIENE	68.118	132.35	317.22	499.00	37.40	276.0	0.2468	0.249	0.147
20	C5H8	trans-1-3-PENTADIENE	68.118	185.71	315.17	500.00	37.40	276.0	0.2468	0.248	0.116
21	C5H8	1-4-PENTADIENE	68.118	124.86	299.11	479.00	37.40	303.0	0.2248	0.285	0.084
22	C5H8	2-3-PENTADIENE	68.118	147.50	321.40	497.00	38.00	295.0	0.2309	0.271	0.218
23	C5H8	1-PENTYNE	68.118	167.45	313.33	481.20	41.70	277.0	0.2459	0.289	0.290
24	C5H8	3-METHYL-1-BUTYNE	68.118	183.45	302.15	463.20	42.00	275.0	0.2477	0.300	0.308
25	C5H8N4O12	PENTAERYTHRITOL TETRANITRATE	316.138	413.65	543.00	676.00	22.40	731.0	0.4325	0.291	1.451
26	C5H8O	CYCLOPENTANONE	84.118	221.85	403.80	626.00	58.50	258.0	0.3260	0.290	0.388
27	C5H8O	METHYL ISOPROPENYL KETONE	84.118	219.55	371.15	566.00	38.90	302.0	0.2785	0.250	0.286
28	C5H8O2	ACETYLACETONE	100.117	249.65	413.55	602.00	39.60	323.0	0.3100	0.256	0.496
29	C5H8O2	ALLYL ACETATE	100.117	138.00	377.15	559.00	36.80	323.0	0.3100	0.256	0.388
30	C5H8O2	ETHYL ACRYLATE	100.117	201.95	372.65	553.00	36.80	323.0	0.3100	0.259	0.378
31	C5H8O2	METHYL METHACRYLATE	100.117	224.95	373.45	564.00	36.80	323.0	0.3100	0.253	0.317
32	C5H8O2	VINYL PROPIONATE	100.117	---	364.35	546.00	36.80	323.0	0.3100	0.262	0.336
33	C5H8O3	2-HYDROXYETHYL ACRYLATE	116.117	213.00	484.00	662.00	39.80	359.0	0.3234	0.260	0.864
34	C5H8O3	LEVULINIC ACID	116.117	308.15	518.95	723.00	40.20	343.0	0.3385	0.229	0.787
35	C5H8O3	METHYL ACETOACETATE	116.117	193.15	444.85	642.00	37.10	343.0	0.3385	0.238	0.513
36	C5H8O4	GLUTARIC ACID	132.116	370.65	595.54	807.00	40.40	363.0	0.3640	0.219	0.959
37	C5H9N	VALERONITRILE	83.133	176.95	414.45	603.00	32.60	331.0	0.2512	0.215	0.415
38	C5H9NO	n-BUTYL ISOCYANATE	99.133	---	388.15	568.00	34.40	360.0	0.2754	0.262	0.415
39	C5H9NO	N-METHYL-2-PYRROLIDONE	99.133	249.15	475.15	724.00	47.80	316.0	0.3137	0.251	0.358
40	C5H9NO4	L-GLUTAMIC ACID	147.131	497.15	670.00	886.00	41.34	383.3	0.3839	0.215	1.197
41	C5H10	CYCLOPENTANE	70.134	179.31	322.40	511.76	45.02	258.3	0.2715	0.273	0.194
42	C5H10	2-METHYL-1-BUTENE	70.134	135.58	304.30	465.00	34.00	292.0	0.2402	0.257	0.229
43	C5H10	2-METHYL-2-BUTENE	70.134	139.39	311.71	471.00	34.00	292.0	0.2402	0.254	0.277
44	C5H10	3-METHYL-1-BUTENE	70.134	104.66	293.21	450.37	35.16	302.1	0.2322	0.284	0.229
45	C5H10	1-PENTENE	70.134	107.93	303.11	464.78	35.29	296.0	0.2369	0.270	0.233
46	C5H10	cis-2-PENTENE	70.134	121.75	310.08	475.93	36.54	302.1	0.2322	0.279	0.241
47	C5H10	trans-2-PENTENE	70.134	132.89	309.49	475.37	36.54	302.1	0.2322	0.279	0.237
48	C5H10Cl2	1-5-DICHLOROPENTANE	141.040	200.35	453.15	663.00	31.90	422.0	0.3342	0.244	0.385
49	C5H10O	METHYL ISOPROPYL KETONE	86.134	181.15	367.55	553.00	38.50	310.0	0.2779	0.260	0.350
50	C5H10O	2-PENTANONE	86.134	196.29	375.46	561.08	36.94	301.0	0.2862	0.238	0.346
51	C5H10O	DIETHYL KETONE	86.134	234.18	375.14	560.95	37.39	336.0	0.2564	0.269	0.350
52	C5H10O	VALERALDEHYDE	86.134	182.00	376.15	554.00	35.00	316.0	0.2726	0.240	0.393
53	C5H10O2	n-BUTYL FORMATE	102.133	181.25	379.25	559.00	35.10	336.0	0.3040	0.254	0.384
54	C5H10O2	ETHYL PROPIONATE	102.133	199.25	372.25	546.00	33.62	345.0	0.2960	0.256	0.394
55	C5H10O2	ISOBUTYL FORMATE	102.133	177.35	371.22	551.35	38.81	352.0	0.2902	0.298	0.390
56	C5H10O2	ISOPROPYL ACETATE	102.133	199.75	361.65	538.00	35.80	336.0	0.3040	0.269	0.355
57	C5H10O2	n-PROPYL ACETATE	102.133	178.15	374.65	549.40	33.60	345.0	0.2960	0.254	0.394
58	C5H10O2	METHYL n-BUTYRATE	102.133	187.35	375.90	554.50	34.73	340.0	0.3004	0.256	0.381
59	C5H10O2	2-METHYLBUTYRIC ACID	102.133	---	450.15	643.00	38.90	347.0	0.2943	0.252	0.589
60	C5H10O2	ISOVALERIC ACID	102.133	243.85	448.25	634.00	38.90	336.0	0.3040	0.248	0.648
61	C5H10O2	VALERIC ACID	102.133	239.15	458.65	651.00	38.10	336.0	0.3040	0.237	0.627
62	C5H10O2	TETRAHYDROFURFURYL ALCOHOL	102.133	---	451.15	639.00	46.60	290.0	0.3522	0.254	0.703
63	C5H10O2S	3-METHYL SULFOLANE	134.199	273.65	549.15	817.00	42.40	353.0	0.3802	0.220	0.419
64	C5H10O3	DIETHYL CARBONATE	118.133	230.15	399.95	576.00	33.90	356.0	0.3318	0.252	0.485
65	C5H10O3	ETHYL LACTATE	118.133	247.15	427.65	588.00	38.60	354.0	0.3337	0.280	0.793

NO	FORMULA	NAME	MW g/mol	T _F K	T _B K	T _C K	P _C bar	V _C cm ³ /mol	ρ _C g/cm ³	Z _C	ω
66	C5H11Cl	1-CHLOROPENTANE	106.595	174.15	381.54	568.00	33.50	352.0	0.3028	0.250	0.334
67	C5H11N	N-METHYLPYRROLIDINE	85.149	183.15	352.30	550.00	42.00	298.0	0.2857	0.274	0.227
68	C5H11N	PIPERIDINE	85.149	262.65	379.55	594.05	46.51	308.0	0.2765	0.290	0.243
69	C5H11NO	tert-BUTYLFORMAMIDE	101.148	289.15	475.15	692.00	35.60	383.0	0.2641	0.237	0.449
70	C5H12	ISOPENTANE	72.150	113.25	300.99	460.43	33.81	305.8	0.2359	0.270	0.228
71	C5H12	NEOPENTANE	72.150	256.58	282.65	433.78	31.99	303.6	0.2377	0.269	0.196
72	C5H12	n-PENTANE	72.150	143.42	309.22	469.65	33.69	312.3	0.2310	0.269	0.249
73	C5H12O	2-2-DIMETHYL-1-PROPANOL	88.150	327.15	386.25	550.00	38.80	327.0	0.2696	0.277	0.604
74	C5H12O	2-METHYL-1-BUTANOL	88.150	---	401.85	565.00	38.80	327.0	0.2696	0.270	0.678
75	C5H12O	2-METHYL-2-BUTANOL	88.150	264.35	375.15	545.15	38.80	327.0	0.2696	0.280	0.483
76	C5H12O	3-METHYL-1-BUTANOL	88.150	155.95	404.35	579.45	38.80	327.0	0.2696	0.263	0.556
77	C5H12O	3-METHYL-2-BUTANOL	88.150	---	386.65	574.00	39.60	327.0	0.2696	0.271	0.351
78	C5H12O	1-PENTANOL	88.150	195.56	410.95	586.15	38.80	326.0	0.2704	0.260	0.594
79	C5H12O	2-PENTANOL	88.150	200.00	392.15	552.00	38.80	327.0	0.2696	0.276	0.675
80	C5H12O	3-PENTANOL	88.150	204.15	388.45	547.00	38.80	327.0	0.2696	0.279	0.675
81	C5H12O	METHYL sec-BUTYL ETHER	88.150	---	332.15	498.00	34.10	329.0	0.2679	0.271	0.306
82	C5H12O	METHYL tert-BUTYL ETHER	88.150	164.55	328.35	497.10	34.30	329.0	0.2679	0.273	0.267
83	C5H12O	METHYL ISOBUTYL ETHER	88.150	---	331.70	497.00	34.10	329.0	0.2679	0.272	0.310
84	C5H12O	ETHYL PROPYL ETHER	88.150	145.65	337.01	500.23	33.70	339.0	0.2600	0.275	0.346
85	C5H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	104.149	183.15	424.50	582.00	36.70	347.0	0.3001	0.263	0.783
86	C5H12O2	NEOPENTYL GLYCOL	104.149	400.00	483.00	643.00	42.40	345.0	0.3019	0.274	1.143
87	C5H12O2	1-5-PENTANEDIOL	104.149	257.15	512.15	673.00	41.50	345.0	0.3019	0.256	1.220
88	C5H12O3	2-(2-METHOXYETHOXY)ETHANOL	120.148	197.15	466.75	630.00	35.40	367.0	0.3274	0.248	0.870
89	C5H12O4	PENTAERYTHRITOL	136.148	534.15	631.00	780.00	47.80	381.0	0.3573	0.281	2.120
90	C5H12S	n-PENTYL MERCAPTAN	104.216	197.45	399.79	598.00	34.70	359.0	0.2903	0.251	0.321
91	C5H13N	n-PENTYLAMINE	87.165	218.15	377.65	555.00	35.80	365.0	0.2388	0.283	0.407
92	C5H13NO2	METHYL DIETHANOLAMINE	119.164	252.15	520.15	678.00	38.80	401.0	0.2972	0.276	1.302
93	C6Cl6	HEXACHLOROBENZENE	284.782	501.70	582.55	825.00	28.50	526.0	0.5414	0.219	0.497
94	C6F6	HEXAFLUOROBENZENE	186.056	278.25	353.41	516.73	32.73	335.0	0.5554	0.255	0.395
95	C6H3ClN2O4	1-CHLORO-2-4-DINITROBENZENE	202.554	326.55	588.00	813.77	34.90	478.0	0.4238	0.247	0.732
96	C6H3Cl2N2O2	1-2-DICHLORO-4-NITROBENZENE	192.001	315.65	529.00	758.00	36.00	436.0	0.4404	0.249	0.539
97	C6H3Cl3	1-2-4-TRICHLOROBENZENE	181.448	290.15	486.15	725.00	37.20	395.0	0.4594	0.244	0.358
98	C6H3N3O6	1-3-5-TRINITROBENZENE	213.106	398.40	748.00	1005.00	33.90	520.0	0.4098	0.211	0.808
99	C6H4Br2	m-DIBROMOBENZENE	235.906	266.25	491.15	761.00	46.60	372.0	0.6342	0.274	0.293
100	C6H4ClNO2	m-CHLORONITROBENZENE	157.556	317.65	508.75	742.00	39.80	432.0	0.3647	0.279	0.489
101	C6H4ClNO2	o-CHLORONITROBENZENE	157.556	306.15	519.00	757.00	39.80	432.0	0.3647	0.273	0.483
102	C6H4ClNO2	p-CHLORONITROBENZENE	157.556	356.65	515.15	751.00	39.80	432.0	0.3647	0.275	0.491
103	C6H4Cl2	m-DICHLOROBENZENE	147.003	248.39	446.23	683.95	40.70	351.0	0.4188	0.251	0.279
104	C6H4Cl2	o-DICHLOROBENZENE	147.003	256.15	453.57	705.00	40.70	351.0	0.4188	0.244	0.219
105	C6H4Cl2	p-DICHLOROBENZENE	147.003	326.14	447.21	684.75	40.70	351.0	0.4188	0.251	0.285
106	C6H4N2O4	m-DINITROBENZENE	168.109	364.00	573.00	805.00	38.50	434.0	0.3873	0.250	0.682
107	C6H4N2O4	o-DINITROBENZENE	168.109	390.08	592.00	831.00	38.50	434.0	0.3873	0.242	0.687
108	C6H4N2O4	p-DINITROBENZENE	168.109	446.60	572.00	803.00	38.50	434.0	0.3873	0.250	0.686
109	C6H5Br	BROMOBENZENE	157.010	242.43	429.24	670.15	45.19	324.0	0.4846	0.263	0.251
110	C6H5Cl	MONOCHLOROBENZENE	112.558	227.95	404.87	632.35	45.19	308.0	0.3654	0.265	0.251
111	C6H5ClO	m-CHLOROPHENOL	128.558	306.00	487.00	729.00	53.20	320.0	0.4017	0.281	0.486
112	C6H5ClO	o-CHLOROPHENOL	128.558	282.00	447.53	675.00	50.00	325.0	0.3956	0.290	0.437
113	C6H5ClO	p-CHLOROPHENOL	128.558	316.00	493.11	738.00	53.20	325.0	0.3956	0.282	0.485
114	C6H5Cl2N	3-4-DICHLOROANILINE	162.018	344.65	545.00	800.00	41.10	409.0	0.3961	0.253	0.468
115	C6H5F	FLUOROBENZENE	96.104	230.94	357.88	560.09	45.51	269.0	0.3573	0.263	0.247
116	C6H5I	IODOBENZENE	204.010	241.83	461.60	721.15	45.19	351.0	0.5812	0.265	0.247
117	C6H5NO2	NITROBENZENE	123.111	278.91	483.95	719.00	44.00	349.0	0.3528	0.257	0.448
118	C6H6	BENZENE	78.114	278.68	353.24	562.16	48.98	258.9	0.3017	0.271	0.211
119	C6H6ClN	m-CHLOROANILINE	127.573	262.75	501.65	751.00	45.90	364.0	0.3505	0.268	0.420
120	C6H6ClN	o-CHLOROANILINE	127.573	481.99	481.99	722.00	45.90	364.0	0.3505	0.278	0.425
121	C6H6ClN	p-CHLOROANILINE	127.573	343.05	503.65	754.00	45.90	364.0	0.3505	0.267	0.421
122	C6H6N2	cis-DICYANO-1-BUTENE	106.127	249.00	501.00	691.00	29.50	392.0	0.2707	0.201	0.672
123	C6H6N2	trans-DICYANO-1-BUTENE	106.127	260.00	499.00	689.00	29.50	392.0	0.2707	0.202	0.664
124	C6H6N2	1-4-DICYANO-2-BUTENE	106.127	349.00	547.00	755.00	29.50	426.0	0.2491	0.200	0.667
125	C6H6N2O2	m-NITROANILINE	138.126	387.15	579.00	815.00	44.20	406.0	0.3402	0.265	0.740
126	C6H6N2O2	o-NITROANILINE	138.126	344.65	558.00	784.00	44.20	406.0	0.3402	0.275	0.741
127	C6H6N2O2	p-NITROANILINE	138.126	420.65	609.15	851.00	44.20	406.0	0.3402	0.254	0.782
128	C6H6O	PHENOL	94.113	314.06	454.99	694.25	61.30	229.0	0.4110	0.243	0.426
129	C6H6O2	1-2-BENZENEDIOL	110.112	377.60	518.65	764.00	74.90	300.0	0.3670	0.354	0.701
130	C6H6O2	1-3-BENZENEDIOL	110.112	382.00	549.65	810.00	74.90	300.0	0.3670	0.334	0.677
131	C6H6O2	p-HYDROQUINONE	110.112	444.65	558.15	822.00	74.50	300.0	0.3670	0.327	0.686
132	C6H6O3	1-2-3-BENZENETRIOL	126.112	407.00	581.85	830.00	88.10	318.0	0.3966	0.406	0.945
133	C6H6S	PHENYL MERCAPTAN	110.180	258.26	442.29	689.00	47.40	315.0	0.3498	0.261	0.263
134	C6H7N	ANILINE	93.128	267.13	457.60	699.00	53.09	270.0	0.3449	0.247	0.404
135	C6H7N	2-METHYLPYRIDINE	93.128	206.44	402.55	621.00	43.80	320.0	0.2910	0.271	0.278
136	C6H7N	3-METHYLPYRIDINE	93.128	255.01	417.29	645.00	43.80	320.0	0.2910	0.261	0.271
137	C6H7N	4-METHYLPYRIDINE	93.128	276.73	418.50	646.15	46.61	325.6	0.2860	0.283	0.302
138	C6H8	1-3-CYCLOHEXADIENE	80.130	161.00	353.49	558.00	47.30	277.0	0.2893	0.282	0.231
139	C6H8	METHYLCYCLOPENTADIENE	80.130	---	345.93	541.00	44.30	279.0	0.2872	0.275	0.238
140	C6H8N2	ADIPONITRILE	108.143	275.64	568.15	781.00	28.30	406.0	0.2664	0.177	0.672
141	C6H8N2	METHYLGUTARONITRILE	108.143	228.15	536.15	742.00	28.80	404.0	0.2677	0.189	0.638

NO	FORMULA	NAME	MW g/mol	T _F K	T _B K	T _C K	P _C bar	V _g cm ³ /mol	ρ _C g/cm ³	Z _C	ω
142	C6H8N2	m-PHENYLENEDIAMINE	108.143	334.00	560.00	824.00	51.80	377.0	0.2869	0.285	0.543
143	C6H8N2	o-PHENYLENEDIAMINE	108.143	376.95	525.00	781.00	51.80	315.0	0.3433	0.251	0.494
144	C6H8N2	p-PHENYLENEDIAMINE	108.143	413.00	540.00	796.00	51.80	317.0	0.3411	0.248	0.539
145	C6H8N2	PHENYLHYDRAZINE	108.143	292.35	516.65	761.00	49.10	418.0	0.2587	0.324	0.535
146	C6H8N2O	BIS(CYANOETHYL)ETHER	124.142	246.85	579.00	783.00	28.30	377.0	0.3293	0.164	0.782
147	C6H8O4	DIMETHYL MALEATE	144.127	254.15	478.15	675.00	32.20	403.0	0.3576	0.231	0.562
148	C6H8O6	ASCORBIC ACID	176.126	465.15	637.00	783.00	52.90	339.0	0.5195	0.275	2.389
149	C6H8O7	CITRIC ACID	192.125	426.15	659.00	822.00	37.98	419.7	0.4578	0.233	1.857
150	C6H10	CYCLOHEXENE	82.145	169.67	356.12	560.40	43.50	291.0	0.2823	0.272	0.214
151	C6H10	2-3-DIMETHYL-1-3-BUTADIENE	82.145	197.15	341.93	526.00	35.20	315.0	0.2608	0.254	0.214
152	C6H10	1-5-HEXADIENE	82.145	132.47	332.61	507.00	33.50	339.0	0.2423	0.269	0.232
153	C6H10	cis-trans-2-4-HEXADIENE	82.145	177.05	356.65	538.00	33.50	331.0	0.2482	0.248	0.275
154	C6H10	trans-trans-2-4-HEXADIENE	82.145	228.25	355.05	535.00	33.50	331.0	0.2482	0.249	0.282
155	C6H10	1-HEXYNE	82.145	141.25	344.48	516.20	36.20	322.0	0.2551	0.272	0.333
156	C6H10	2-HEXYNE	82.145	183.65	357.67	549.00	35.30	331.0	0.2482	0.256	0.221
157	C6H10	3-HEXYNE	82.145	170.05	354.35	544.00	35.30	331.0	0.2482	0.258	0.218
158	C6H10O	CYCLOHEXANONE	98.145	242.00	428.90	629.15	38.50	311.0	0.3156	0.229	0.450
159	C6H10O	MESITYL OXIDE	98.145	220.15	402.95	600.00	34.10	355.0	0.2765	0.243	0.327
160	C6H10O2	epsilon-CAPROLACTONE	114.144	271.85	514.00	771.00	46.30	352.0	0.3243	0.254	0.442
161	C6H10O2	ETHYL METHACRYLATE	114.144	---	390.15	577.00	32.50	375.0	0.3044	0.254	0.344
162	C6H10O2	n-PROPYL ACRYLATE	114.144	---	392.15	569.00	32.50	376.0	0.3036	0.258	0.434
163	C6H10O3	ETHYLACETOACETATE	130.144	234.15	453.95	643.00	32.70	391.0	0.3328	0.239	0.561
164	C6H10O3	PROPIONIC ANHYDRIDE	130.144	228.15	442.15	618.00	33.40	396.0	0.3286	0.257	0.618
165	C6H10O4	ADIPIC ACID	146.143	425.50	611.00	809.00	35.30	400.0	0.3654	0.210	1.054
166	C6H10O4	DIETHYL OXALATE	146.143	232.55	458.85	646.00	30.90	416.0	0.3513	0.239	0.568
167	C6H10O4	ETHYLENE GLYCOL DIACETATE	146.143	242.15	463.65	653.00	30.90	416.0	0.3513	0.237	0.560
168	C6H10O4	ETHYLIDENE DIACETATE	146.143	292.00	442.15	635.00	32.60	406.0	0.3600	0.251	0.478
169	C6H11N	HEXANENITRILE	97.160	192.85	436.75	622.05	29.20	384.0	0.2530	0.217	0.474
170	C6H11NO	epsilon-CAPROLACTAM	113.159	342.36	543.15	806.00	47.70	356.0	0.3179	0.253	0.477
171	C6H11NO	CYCLOHEXANONE OXIME	113.159	363.15	481.15	715.00	46.90	369.0	0.3067	0.291	0.462
172	C6H12	CYCLOHEXANE	84.161	279.69	353.87	553.54	40.75	307.9	0.2734	0.273	0.212
173	C6H12	2-3-DIMETHYL-1-BUTENE	84.161	115.89	328.76	500.00	32.20	349.0	0.2411	0.270	0.227
174	C6H12	2-3-DIMETHYL-2-BUTENE	84.161	198.82	346.35	524.00	31.60	372.0	0.2262	0.270	0.233
175	C6H12	3-3-DIMETHYL-1-BUTENE	84.161	157.95	314.40	480.00	32.90	333.0	0.2527	0.275	0.226
176	C6H12	2-ETHYL-1-BUTENE	84.161	141.61	337.82	512.00	31.60	364.0	0.2312	0.270	0.228
177	C6H12	1-HEXENE	84.161	133.39	336.63	504.03	31.40	354.0	0.2377	0.265	0.280
178	C6H12	cis-2-HEXENE	84.161	132.00	342.03	513.00	31.60	359.0	0.2344	0.266	0.272
179	C6H12	trans-2-HEXENE	84.161	140.17	341.02	513.00	31.60	360.0	0.2338	0.267	0.261
180	C6H12	cis-3-HEXENE	84.161	135.33	339.60	509.00	31.70	351.0	0.2398	0.263	0.279
181	C6H12	trans-3-HEXENE	84.161	159.73	340.24	509.00	31.70	351.0	0.2398	0.263	0.285
182	C6H12	METHYLCYCLOPENTANE	84.161	130.73	344.96	532.79	37.85	318.9	0.2639	0.272	0.230
183	C6H12	2-METHYL-1-PENTENE	84.161	137.42	335.25	507.00	31.60	359.0	0.2344	0.269	0.241
184	C6H12	2-METHYL-2-PENTENE	84.161	138.07	340.45	514.00	31.60	363.0	0.2318	0.268	0.245
185	C6H12	3-METHYL-1-PENTENE	84.161	120.20	327.33	495.00	32.90	343.3	0.2452	0.274	0.264
186	C6H12	3-METHYL-cis-2-PENTENE	84.161	138.31	340.85	515.00	32.90	343.0	0.2454	0.264	0.259
187	C6H12	4-METHYL-1-PENTENE	84.161	119.51	327.01	496.00	32.20	345.0	0.2439	0.269	0.239
188	C6H12	4-METHYL-cis-2-PENTENE	84.161	138.30	329.53	499.00	32.20	346.0	0.2432	0.269	0.244
189	C6H12	4-METHYL-trans-2-PENTENE	84.161	132.35	331.75	501.00	32.20	346.0	0.2432	0.267	0.255
190	C6H12N2	TRIETHYLENEDIAMINE	112.175	434.25	447.15	655.00	39.10	382.0	0.2937	0.274	0.460
191	C6H12O	BUTYL VINYL ETHER	100.161	181.25	366.97	536.00	31.20	364.0	0.2752	0.255	0.380
192	C6H12O	CYCLOHEXANOL	100.161	296.60	434.00	625.15	37.49	322.0	0.3111	0.232	0.514
193	C6H12O	1-HEXANAL	100.161	217.15	401.45	579.00	31.10	369.0	0.2714	0.238	0.439
194	C6H12O	ETHYL ISOPROPYL KETONE	100.161	---	386.55	567.00	33.20	369.0	0.2714	0.260	0.391
195	C6H12O	2-HEXANONE	100.161	217.35	400.85	587.05	33.24	369.0	0.2714	0.251	0.397
196	C6H12O	3-HEXANONE	100.161	217.50	396.65	582.82	33.20	364.0	0.2752	0.249	0.376
197	C6H12O	METHYL ISOBUTYL KETONE	100.161	189.15	389.65	571.40	32.73	369.0	0.2714	0.254	0.389
198	C6H12O2	n-PENTYL FORMATE	116.160	199.65	406.60	576.00	31.25	389.0	0.2986	0.254	0.528
199	C6H12O2	n-BUTYL ACETATE	116.160	199.65	399.15	579.65	31.10	389.0	0.2986	0.251	0.410
200	C6H12O2	sec-BUTYL ACETATE	116.160	174.15	385.15	561.00	31.70	389.0	0.2986	0.264	0.406
201	C6H12O2	tert-BUTYL ACETATE	116.160	---	369.15	545.00	31.70	389.0	0.2986	0.272	0.343
202	C6H12O2	ETHYL n-BUTYRATE	116.160	175.15	394.65	571.00	30.60	421.0	0.2759	0.271	0.419
203	C6H12O2	ETHYL ISOBUTYRATE	116.160	185.00	383.00	553.15	30.40	410.0	0.2833	0.271	0.426
204	C6H12O2	ISOBUTYL ACETATE	116.160	174.30	389.80	561.00	31.60	389.0	0.2986	0.264	0.454
205	C6H12O2	n-PROPYL PROPIONATE	116.160	197.25	395.65	578.00	31.10	389.0	0.2986	0.252	0.376
206	C6H12O2	CYCLOHEXYL PEROXIDE	116.160	253.15	490.00	685.00	42.10	342.0	0.3396	0.253	0.751
207	C6H12O2	DIACETONE ALCOHOL	116.160	229.15	441.00	606.00	36.00	387.0	0.3002	0.277	0.757
208	C6H12O2	2-ETHYL BUTYRIC ACID	116.160	258.15	466.95	655.00	34.10	389.0	0.2986	0.244	0.633
209	C6H12O2	n-HEXANOIC ACID	116.160	270.15	478.85	667.00	33.50	389.0	0.2986	0.235	0.670
210	C6H12O3	2-ETHOXYETHYL ACETATE	132.159	211.45	429.45	597.00	24.62	409.0	0.3231	0.203	0.534
211	C6H12O3	HYDROXYCAPROIC ACID	132.159	334.00	576.00	758.00	36.40	402.0	0.3288	0.232	1.163
212	C6H12O3	PARALDEHYDE	132.159	285.75	397.25	579.00	35.00	365.0	0.3621	0.265	0.441
213	C6H12O3	sec-BUTYL GLYCOLATE	132.160	---	450.65	---	---	---	---	---	---
214	C6H13N	CYCLOHEXYLAMINE	99.176	255.45	407.65	615.00	42.00	360.0	0.2755	0.296	0.360
215	C6H13N	HEXAMETHYLENEIMINE	99.176	236.15	404.85	615.00	42.70	361.0	0.2747	0.301	0.330
216	C6H14	2-2-DIMETHYLBUTANE	86.177	174.28	322.88	488.78	30.81	358.8	0.2402	0.272	0.234
217	C6H14	2-3-DIMETHYLBUTANE	86.177	145.19	331.13	499.98	31.27	357.8	0.2409	0.269	0.248

NO	FORMULA	NAME	MW g/mol	T _F K	T _B K	T _C K	P _C bar	V _C cm ³ /mol	ρ _C g/cm ³	Z _C	ω
218	C6H14	n-HEXANE	86.177	177.84	341.88	507.43	30.12	369.9	0.2330	0.264	0.305
219	C6H14	2-METHYLPENTANE	86.177	119.55	333.41	497.50	30.10	366.4	0.2352	0.267	0.278
220	C6H14	3-METHYLPENTANE	86.177	110.25	336.42	504.43	31.24	366.4	0.2352	0.273	0.274
221	C6H14N2O2	LYSINE	146.189	483.00	615.00	821.00	35.30	502.0	0.2912	0.260	1.012
222	C6H14O	2-ETHYL-1-BUTANOL	102.177	158.75	419.65	580.00	34.00	380.0	0.2689	0.268	0.714
223	C6H14O	1-HEXANOL	102.177	228.55	430.15	611.35	35.10	381.3	0.2680	0.263	0.580
224	C6H14O	2-HEXANOL	102.177	223.00	413.04	586.20	34.00	380.0	0.2689	0.265	0.566
225	C6H14O	2-METHYL-1-PENTANOL	102.177	---	421.15	582.00	34.00	380.0	0.2689	0.267	0.726
226	C6H14O	4-METHYL-2-PENTANOL	102.177	---	404.85	574.40	34.70	380.0	0.2689	0.276	0.572
227	C6H14O	n-BUTYL ETHYL ETHER	102.177	170.15	365.35	531.00	29.90	382.0	0.2675	0.259	0.390
228	C6H14O	DIISOPROPYL ETHER	102.177	187.65	341.45	500.05	28.78	386.0	0.2647	0.267	0.338
229	C6H14O	DI-n-PROPYL ETHER	102.177	149.95	362.79	530.60	30.28	382.0	0.2675	0.262	0.370
230	C6H14O	METHYL tert-PENTYL ETHER	102.177	---	359.45	534.00	30.40	382.0	0.2675	0.262	0.301
231	C6H14O2	ACETAL	118.176	173.15	376.75	541.00	29.80	402.0	0.2940	0.266	0.432
232	C6H14O2	2-BUTOXYETHANOL	118.176	203.15	444.47	600.00	32.40	400.0	0.2954	0.260	0.817
233	C6H14O2	1-6-HEXANEDIOL	118.176	315.15	516.15	670.00	36.10	398.0	0.2969	0.258	1.268
234	C6H14O2	HEXYLENE GLYCOL	118.176	223.15	470.65	621.00	40.10	398.0	0.2969	0.309	1.197
235	C6H14O2S	DI-n-PROPYL SULFONE	150.242	303.00	543.00	763.00	31.10	463.0	0.3245	0.227	0.582
236	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	134.175	203.15	432.91	604.00	28.60	422.0	0.3180	0.240	0.575
237	C6H14O3	DIPROPYLENE GLYCOL	134.175	233.00	504.95	654.00	35.80	415.0	0.3233	0.273	1.198
238	C6H14O3	2-(2-ETHOXYETHOXY)ETHANOL	134.175	195.15	475.15	632.00	31.40	420.0	0.3195	0.251	0.901
239	C6H14O3	TRIMETHYLOLPROPANE	134.175	331.15	562.04	709.00	39.10	416.0	0.3225	0.276	1.543
240	C6H14O4	TRIETHYLENE GLYCOL	150.175	265.79	551.00	700.00	33.20	443.0	0.3390	0.253	1.386
241	C6H14O6	SORBITOL	182.174	370.85	777.00	959.00	46.40	483.0	0.3772	0.281	2.199
242	C6H14S	n-HEXYLMERCAPTAN	118.243	192.62	425.81	623.00	30.80	412.0	0.2870	0.245	0.368
243	C6H15Al	TRIETHYL ALUMINUM	114.167	220.65	458.15	720.15	13.58	230.0	0.4964	0.522	---
244	C6H15Al2Cl3	ETHYL ALUMINUM SESQUICHLORIDE	247.506	253.15	482.15	791.00	---	---	---	---	---
245	C6H15N	DIISOPROPYLAMINE	101.192	176.85	357.05	523.10	32.00	418.0	0.2421	0.308	0.388
246	C6H15N	DI-n-PROPYLAMINE	101.192	210.15	382.00	555.80	36.30	418.0	0.2421	0.328	0.465
247	C6H15N	n-HEXYLAMINE	101.192	251.85	404.65	583.00	31.80	418.0	0.2421	0.274	0.467
248	C6H15N	TRIETHYLAMINE	101.192	158.45	361.92	535.15	30.40	390.0	0.2595	0.266	0.316
249	C6H15NO	6-AMINOHEXANOL	117.191	331.00	508.00	681.00	34.40	436.0	0.2688	0.265	0.970
250	C6H15NO2	DIISOPROPANOLAMINE	133.191	318.15	521.90	672.00	36.00	454.0	0.2934	0.293	1.389
251	C6H15NO3	TRIETHANOLAMINE	149.190	294.35	613.00	787.00	24.50	472.0	0.3161	0.177	1.101
252	C6H15N3	N-AMINOETHYL PIPERAZINE	129.205	254.15	493.55	708.00	38.50	407.0	0.3175	0.266	0.555
253	C6H15O4P	TRIETHYL PHOSPHATE	182.156	216.00	484.15	794.00	10.80	1010.0	0.1804	1.650	---
254	C6H16N2	HEXAMETHYLENEDIAMINE	116.207	313.95	475.04	663.00	32.90	475.0	0.2446	0.284	0.650
255	C6H18N3OP	HEXAMETHYL PHOSPHORAMIDE	179.202	280.15	506.15	---	---	---	---	---	---
256	C6H18N4	TRIETHYLENE TETRAMINE	146.236	285.15	539.65	718.00	31.70	482.0	0.3034	0.256	0.974
257	C6H18OSi2	HEXAMETHYLDISILOXANE	162.379	204.93	373.67	518.70	19.14	601.0	0.2702	0.267	0.418
258	C6H18O3Si3	HEXAMETHYLCYCLOTRISILOXANE	222.464	337.15	408.26	554.20	16.63	634.0	0.3509	0.229	0.474
259	C6H19NSi2	HEXAMETHYLDISILAZANE	161.395	---	399.15	544.00	19.20	613.0	0.2633	0.260	0.510
260	C7H3ClF3NO24	CHLORO-3-NITROBENZOTRIFLUORIDE	225.554	---	495.15	686.00	27.40	490.0	0.4603	0.235	0.607
261	C7H3Cl2F3	2-4-DICHLOROBENZOTRIFLUORIDE	215.001	247.55	450.65	646.00	28.10	443.0	0.4853	0.232	0.434
262	C7H3Cl2NO	3-4-DICHLOROPHENYL ISOCYANATE	188.012	316.15	501.00	733.00	33.30	456.0	0.4123	0.249	0.335
263	C7H4ClF3	p-CHLOROBENZOTRIFLUORIDE	180.557	237.15	412.15	601.00	30.10	399.0	0.4525	0.240	0.373
264	C7H4Cl2O	m-CHLOROBENZYL CHLORIDE	175.014	280.00	498.00	724.00	36.80	406.0	0.4311	0.248	0.454
265	C7H4F3NO2	3-NITROBENZOTRIFLUORIDE	191.110	272.00	475.93	667.00	28.00	441.0	0.4334	0.223	0.536
266	C7H5ClO	BENZYL CHLORIDE	140.569	272.65	470.15	697.00	40.60	367.0	0.3830	0.257	0.421
267	C7H5ClO2	o-CHLOROBENZOIC ACID	156.568	415.15	560.15	792.00	40.30	383.0	0.4088	0.234	0.664
268	C7H5Cl3	BENZOTRICHLORIDE	195.475	268.40	486.65	737.00	33.40	447.0	0.4373	0.244	0.260
269	C7H5F3	BENZOTRIFLUORIDE	146.112	244.14	375.20	565.00	33.90	356.0	0.4104	0.257	0.282
270	C7H5N	BENZONITRILE	103.123	260.40	464.15	699.35	42.15	339.0	0.3042	0.246	0.352
271	C7H5NO	PHENYL ISOCYANATE	119.123	243.15	438.75	648.00	40.60	341.0	0.3493	0.257	0.438
272	C7H5N3O6	2-4-6-TRINITROTOLUENE	227.133	354.00	573.00	795.00	30.40	480.0	0.4732	0.221	1.977
273	C7H6Cl2	BENZYL DICHLORIDE	161.030	257.00	487.00	731.00	36.50	404.0	0.3986	0.243	0.326
274	C7H6Cl2	2-4-DICHLOROTOLUENE	161.030	259.65	474.25	705.00	35.90	404.0	0.3986	0.247	0.359
275	C7H6N2O4	2-4-DINITROTOLUENE	182.136	343.00	590.00	814.00	34.00	487.0	0.3740	0.245	0.718
276	C7H6N2O4	2-5-DINITROTOLUENE	182.136	325.65	590.00	814.00	34.00	472.0	0.3859	0.237	0.740
277	C7H6N2O4	2-6-DINITROTOLUENE	182.136	339.00	558.00	770.00	36.00	487.0	0.3740	0.242	0.738
278	C7H6N2O4	3-4-DINITROTOLUENE	182.136	332.00	610.00	842.00	34.00	487.0	0.3740	0.237	0.737
279	C7H6N2O4	3-5-DINITROTOLUENE	182.136	365.65	588.00	814.00	34.00	473.0	0.3851	0.238	0.702
280	C7H6O	BENZALDEHYDE	106.124	247.15	451.90	695.00	46.50	324.0	0.3275	0.261	0.305
281	C7H6O2	BENZOIC ACID	122.123	395.52	522.40	751.00	44.70	339.1	0.3600	0.246	0.604
282	C7H6O2	p-HYDROXYBENZALDEHYDE	122.123	390.15	583.15	844.00	49.90	361.0	0.3383	0.257	0.617
283	C7H6O2	SALICYLALDEHYDE	122.123	266.15	469.65	680.00	49.90	342.0	0.3571	0.302	0.626
284	C7H6O3	SALICYLIC ACID	138.123	431.75	529.00	739.00	51.80	364.0	0.3795	0.307	0.832
285	C7H7Br	p-BROMOTOLUENE	171.037	299.95	457.50	699.00	43.70	379.0	0.4513	0.285	0.318
286	C7H7Cl	BENZYL CHLORIDE	126.585	234.15	452.55	686.00	39.10	360.0	0.3516	0.247	0.314
287	C7H7Cl	o-CHLOROTOLUENE	126.585	236.65	432.30	656.00	39.10	354.0	0.3576	0.254	0.304
288	C7H7Cl	p-CHLOROTOLUENE	126.585	280.65	435.65	660.00	39.10	360.0	0.3516	0.257	0.313
289	C7H7NO	FORMANILIDE	121.139	323.15	544.15	787.00	41.10	382.0	0.3171	0.240	0.545
290	C7H7NO2	m-NITROTOLUENE	137.138	289.20	505.00	734.00	38.00	441.0	0.3110	0.275	0.490
291	C7H7NO2	o-NITROTOLUENE	137.138	269.98	495.64	720.00	38.00	441.0	0.3110	0.280	0.482
292	C7H7NO2	p-NITROTOLUENE	137.138	324.75	511.65	736.00	38.00	441.0	0.3110	0.274	0.541
293	C7H7NO3	o-NITROANISOLE	153.138	283.60	546.15	782.00	37.60	422.0	0.3629	0.244	0.561

NO	FORMULA	NAME	MW g/mol	T _F K	T _B K	T _C K	P _C bar	V _C cm ³ /mol	ρ _C g/cm ³	Z _C	ω
294	C7H8	TOLUENE	92.141	178.18	383.78	591.79	41.09	315.8	0.2918	0.264	0.264
295	C7H8O	ANISOLE	108.140	235.65	426.73	641.65	41.75	337.0	0.3209	0.264	0.369
296	C7H8O	BENZYL ALCOHOL	108.140	257.85	477.85	677.00	45.50	335.0	0.3228	0.271	0.691
297	C7H8O	m-CRESOL	108.140	285.39	475.43	705.85	45.60	312.0	0.3466	0.242	0.449
298	C7H8O	o-CRESOL	108.140	304.19	464.15	697.55	50.06	282.0	0.3835	0.243	0.434
299	C7H8O	p-CRESOL	108.140	307.93	475.13	704.65	51.50	277.0	0.3904	0.244	0.513
300	C7H8O2	GUAIACOL	124.139	304.65	478.15	697.00	47.30	353.0	0.3517	0.288	0.563
301	C7H8O2	p-METHOXYPHENOL	124.139	329.00	516.00	758.00	49.70	342.0	0.3630	0.270	0.541
302	C7H9N	BENZYLAMINE	107.155	227.15	457.65	683.50	43.20	373.0	0.2873	0.284	0.409
303	C7H9N	2-6-DIMETHYLPYRIDINE	107.155	267.00	417.20	623.75	37.80	316.0	0.3391	0.230	0.350
304	C7H9N	N-METHYLANILINE	107.155	216.15	469.02	701.55	51.98	373.0	0.2873	0.332	0.480
305	C7H9N	m-TOLUIDINE	107.155	242.75	476.55	709.15	41.54	373.0	0.2873	0.263	0.413
306	C7H9N	o-TOLUIDINE	107.155	249.47	473.55	694.15	37.49	373.0	0.2873	0.242	0.442
307	C7H9N	p-TOLUIDINE	107.155	316.90	473.40	693.15	40.00	373.0	0.2873	0.259	0.476
308	C7H10	2-NORBORNENE	94.156	319.40	368.65	583.00	39.30	337.0	0.2794	0.273	0.159
309	C7H10N2	TOLUENEDIAMINE	122.170	371.25	557.15	804.00	43.80	376.0	0.3249	0.246	0.576
310	C7H11NO	CYCLOHEXYL ISOCYANATE	125.170	---	442.15	633.00	34.70	408.0	0.3068	0.269	0.530
311	C7H12O2	n-BUTYL ACRYLATE	128.171	208.55	421.00	598.00	26.30	428.0	0.2995	0.226	0.438
312	C7H12O2	ISOBUTYL ACRYLATE	128.171	212.00	405.15	580.00	29.50	428.0	0.2995	0.262	0.457
313	C7H12O2	n-PROPYL METHACRYLATE	128.171	---	414.00	599.00	29.10	428.0	0.2995	0.250	0.401
314	C7H12O4	DIETHYL MALONATE	160.170	224.25	472.05	653.00	27.80	469.0	0.3415	0.240	0.611
315	C7H14	CYCLOHEPTANE	98.188	265.15	391.94	604.30	38.40	359.0	0.2735	0.274	0.243
316	C7H14	1-1-DIMETHYLCYCLOPENTANE	98.188	203.36	361.00	547.00	34.45	360.0	0.2727	0.273	0.272
317	C7H14	cis-1-2-DIMETHYLCYCLOPENTANE	98.188	219.26	372.68	565.15	34.45	370.0	0.2654	0.271	0.266
318	C7H14	trans-1-2-DIMETHYLCYCLOPENTANE	98.188	155.58	365.02	553.15	34.45	360.0	0.2727	0.270	0.270
319	C7H14	cis-1-3-DIMETHYLCYCLOPENTANE	98.188	139.45	363.92	551.00	34.45	360.0	0.2727	0.271	0.274
320	C7H14	trans-1-3-DIMETHYLCYCLOPENTANE	98.188	139.18	364.88	553.00	34.45	360.0	0.2727	0.270	0.270
321	C7H14	ETHYLCYCLOPENTANE	98.188	134.71	376.62	569.52	33.98	374.5	0.2622	0.269	0.272
322	C7H14	2-ETHYL-1-PENTENE	98.188	168.00	367.15	543.00	29.50	398.0	0.2467	0.260	0.309
323	C7H14	3-ETHYL-1-PENTENE	98.188	145.67	357.26	530.00	30.30	398.0	0.2467	0.274	0.302
324	C7H14	1-HEPTENE	98.188	154.27	366.79	537.29	28.30	413.0	0.2377	0.262	0.331
325	C7H14	cis-2-HEPTENE	98.188	164.00	371.56	549.00	28.40	424.0	0.2316	0.264	0.294
326	C7H14	trans-2-HEPTENE	98.188	163.67	371.10	543.00	28.50	406.0	0.2418	0.256	0.337
327	C7H14	cis-3-HEPTENE	98.188	136.51	368.90	545.00	28.40	421.0	0.2332	0.264	0.295
328	C7H14	trans-3-HEPTENE	98.188	136.52	368.82	540.00	28.50	406.0	0.2418	0.258	0.334
329	C7H14	METHYLCYCLOHEXANE	98.188	146.58	374.08	572.19	34.71	368.0	0.2668	0.269	0.235
330	C7H14	2-METHYL-1-HEXENE	98.188	170.28	364.99	538.00	28.70	398.0	0.2467	0.255	0.309
331	C7H14	3-METHYL-1-HEXENE	98.188	145.00	357.05	528.00	29.50	398.0	0.2467	0.267	0.306
332	C7H14	4-METHYL-1-HEXENE	98.188	131.70	359.88	534.00	30.40	398.0	0.2467	0.273	0.302
333	C7H14	2-3-3-TRIMETHYL-1-BUTENE	98.188	163.30	351.04	531.00	31.40	381.0	0.2577	0.270	0.241
334	C7H14O	DIISOPROPYL KETONE	114.188	204.81	397.55	576.00	30.20	416.0	0.2745	0.262	0.405
335	C7H14O	2-HEPTANONE	114.188	238.15	424.05	611.55	29.20	421.0	0.2712	0.242	0.413
336	C7H14O	1-HEPTANAL	114.188	230.15	425.95	603.00	28.00	421.0	0.2712	0.235	0.487
337	C7H14O	1-METHYLCYCLOHEXANOL	114.188	299.15	430.15	603.00	37.90	414.0	0.2758	0.313	0.683
338	C7H14O	cis-2-METHYLCYCLOHEXANOL	114.188	280.15	438.15	614.00	37.90	414.0	0.2758	0.307	0.679
339	C7H14O	trans-2-METHYLCYCLOHEXANOL	114.188	269.15	439.65	616.00	37.90	414.0	0.2758	0.306	0.683
340	C7H14O	cis-3-METHYLCYCLOHEXANOL	114.188	267.65	441.15	618.00	37.90	414.0	0.2758	0.305	0.704
341	C7H14O	trans-3-METHYLCYCLOHEXANOL	114.188	272.65	441.15	617.00	37.90	414.0	0.2758	0.306	0.697
342	C7H14O	cis-4-METHYLCYCLOHEXANOL	114.188	---	444.15	622.00	37.90	414.0	0.2758	0.303	0.658
343	C7H14O	trans-4-METHYLCYCLOHEXANOL	114.188	---	444.15	622.00	37.90	414.0	0.2758	0.303	0.691
344	C7H14O	5-METHYL-2-HEXANONE	114.188	199.25	417.95	601.00	29.70	421.0	0.2712	0.250	0.434
345	C7H14O2	n-BUTYL PROPIONATE	130.187	183.63	419.75	594.00	28.00	442.0	0.2945	0.251	0.475
346	C7H14O2	ETHYL ISOVALERATE	130.187	173.85	407.45	587.95	28.40	442.0	0.2945	0.257	0.407
347	C7H14O2	ISOPENTYL ACETATE	130.187	194.65	415.25	599.00	28.40	442.0	0.2945	0.252	0.414
348	C7H14O2	n-PENTYL ACETATE	130.187	202.35	422.15	598.00	28.00	442.0	0.2945	0.249	0.490
349	C7H14O2	n-PROPYL n-BUTYRATE	130.187	177.95	416.45	594.00	28.00	442.0	0.2945	0.251	0.448
350	C7H14O2	n-HEPTANOIC ACID	130.187	265.83	496.15	680.00	29.90	442.0	0.2945	0.234	0.717
351	C7H14O3	ETHYL-3-ETHOXYPROPIONATE	146.186	---	438.15	609.00	27.20	462.0	0.3164	0.248	0.578
352	C7H15Br	1-BROMOHEPTANE	179.100	217.05	452.05	651.00	30.80	447.0	0.4007	0.271	0.444
353	C7H15N	N-METHYLCYCLOHEXYLAMINE	113.203	264.65	422.00	622.00	34.90	393.0	0.2880	0.265	0.386
354	C7H16	2-2-DIMETHYLPENTANE	100.204	149.34	352.34	520.50	37.73	416.0	0.2409	0.267	0.288
355	C7H16	2-3-DIMETHYLPENTANE	100.204	---	362.93	537.35	29.08	393.0	0.2550	0.256	0.292
356	C7H16	2-4-DIMETHYLPENTANE	100.204	153.91	353.64	519.79	27.37	418.0	0.2397	0.265	0.302
357	C7H16	3-3-DIMETHYLPENTANE	100.204	138.70	359.21	536.40	29.46	414.0	0.2420	0.273	0.267
358	C7H16	3-ETHYLPENTANE	100.204	154.55	366.62	540.64	28.91	416.0	0.2409	0.268	0.309
359	C7H16	n-HEPTANE	100.204	182.57	371.58	540.26	27.36	431.9	0.2320	0.263	0.351
360	C7H16	2-METHYLHEXANE	100.204	154.90	363.20	530.37	27.34	421.0	0.2380	0.261	0.328
361	C7H16	3-METHYLHEXANE	100.204	153.75	365.00	535.25	28.14	404.0	0.2480	0.255	0.322
362	C7H16	2-2-3-TRIMETHYLBUTANE	100.204	248.57	354.03	531.17	29.54	398.0	0.2518	0.266	0.250
363	C7H16O	1-HEPTANOL	116.203	239.15	449.45	631.90	31.50	435.2	0.2670	0.261	0.587
364	C7H16O	2-HEPTANOL	116.203	243.00	432.35	588.00	30.30	432.0	0.2690	0.268	0.763
365	C7H16O	5-METHYL-1-HEXANOL	116.203	---	445.15	605.00	30.30	432.0	0.2690	0.260	0.781
366	C7H16S	n-HEPTYL MERCAPTAN	132.270	229.92	450.09	645.00	27.70	456.0	0.2901	0.240	0.419
367	C7H17N	1-AMINOHEPTANE	115.219	254.15	430.05	607.00	28.50	471.0	0.2446	0.266	0.511

Appendix E

GAS HEAT CAPACITY FOR C₅ TO C₇ COMPOUNDS

Carl L. Yaws
Lamar University, Beaumont, Texas

			$C_p = A + B T + C T^2 + D T^3 + E T^4$ (C _p - joule/g-mol K, T - K)						
NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
1	C5Cl6	HEXACHLOROCYCLOPENTADIENE	38.750	8.0546E-01	-1.5519E-03	1.4183E-06	-4.8251E-10	298	1000
2	C5H4O2	FURFURAL	15.470	2.9835E-01	-1.9177E-05	-1.4621E-07	5.9506E-11	100	1500
3	C5H5N	PYRIDINE	23.262	1.1251E-01	3.7351E-04	-4.5402E-07	1.4286E-10	50	1500
4	C5H6	CYCLOPENTADIENE	-25.616	4.2049E-01	-2.7180E-04	7.2995E-08	-3.9537E-12	200	1500
5	C5H6	2-METHYL-1-BUTENE-3-YNE	11.399	3.4714E-01	-2.3506E-04	7.6877E-08	-9.4000E-12	298	1500
6	C5H6	1-PENTENE-3-YNE	9.264	3.3995E-01	-2.3573E-04	8.8403E-08	-1.4533E-11	298	1500
7	C5H6	1-PENTENE-4-YNE	11.588	3.4489E-01	-2.5839E-04	1.0999E-07	-2.0576E-11	298	1500
8	C5H6N2	GLUTARONITRILE	18.975	3.9760E-01	-2.4793E-04	6.6492E-08	-6.1305E-12	298	1500
9	C5H6O2	FURFURYL ALCOHOL	-7.696	5.5491E-01	-4.9754E-04	2.3193E-07	-4.4815E-11	298	1500
10	C5H6O3	GLUTARIC ANHYDRIDE	-39.768	6.2221E-01	-3.8554E-04	1.0999E-07	-1.1564E-11	298	1500
11	C5H6O4	CITRACONIC ACID	-44.280	9.7863E-01	-1.3251E-03	9.3278E-07	-2.5668E-10	298	1200
12	C5H6O4	ITACONIC ACID	-29.874	8.3391E-01	-1.0039E-03	6.4524E-07	-1.6726E-10	298	1200
13	C5H7N	N-METHYLPYRROLE	-42.333	5.9879E-01	-5.0928E-04	2.4282E-07	-4.8924E-11	298	1500
14	C5H7NO2	ETHYL CYANOACETATE	-28.861	6.9064E-01	-6.7310E-04	3.4241E-07	-7.0338E-11	298	1500
15	C5H8	CYCLOPENTENE	-4.355	2.5989E-01	1.1735E-04	-2.3049E-07	7.6078E-11	200	1500
16	C5H8	ISOPRENE	-0.007	4.2828E-01	-3.0377E-04	1.1890E-07	-2.0653E-11	200	1500
17	C5H8	3-METHYL-1,2-BUTADIENE	33.913	2.2132E-01	4.9559E-05	-1.2900E-07	4.1214E-11	150	1500
18	C5H8	1,2-PENTADIENE	15.041	3.3233E-01	-1.2798E-04	-1.0733E-08	1.3140E-11	200	1500
19	C5H8	cis-1,3-PENTADIENE	11.441	3.2718E-01	-1.0552E-04	-3.1107E-08	1.8831E-11	200	1500
20	C5H8	trans-1,3-PENTADIENE	10.384	3.4613E-01	-1.4819E-04	3.3729E-09	9.3660E-12	200	1500
21	C5H8	1,4-PENTADIENE	28.759	2.2687E-01	1.0259E-04	-1.9453E-07	6.2357E-11	100	1500
22	C5H8	2,3-PENTADIENE	29.678	2.8033E-01	-7.3692E-05	-3.3295E-08	1.5621E-11	150	1500
23	C5H8	1-PENTYNE	18.298	3.5705E-01	-2.0856E-04	5.4791E-08	-4.3208E-12	200	1500
24	C5H8	3-METHYL-1-BUTYNE	33.392	2.6136E-01	-1.6275E-05	-9.4718E-08	3.6363E-11	200	1500
25	C5H8N4O12	PENTAERYTHRITOL TETRANITRATE	-29.270	5.0540E-01	-3.4447E-04	1.3119E-07	-2.6198E-11	298	1500
26	C5H8O	CYCLOPENTANONE	-6.032	4.4160E-01	-2.5697E-04	5.3823E-08	2.4497E-12	298	1200
27	C5H8O	METHYL ISOPROPENYL KETONE	-6.071	5.0469E-01	-3.9471E-04	2.1259E-07	-6.0544E-11	298	1200
28	C5H8O2	ACETYLACETONE	-20.793	6.0941E-01	-5.2082E-04	2.3682E-07	-4.6892E-11	298	1500
29	C5H8O2	ALLYL ACETATE	-9.599	5.4466E-01	-4.1029E-04	1.6344E-07	-3.1021E-11	298	1500
30	C5H8O2	ETHYL ACRYLATE	-25.526	6.0628E-01	-5.0627E-04	2.2388E-07	-4.2286E-11	298	1500
31	C5H8O2	METHYL METHACRYLATE	-1.977	4.8760E-01	-2.8547E-04	4.8284E-08	7.1078E-12	298	1500
32	C5H8O2	VINYL PROPIONATE	-36.842	8.7884E-01	-1.0766E-03	6.9101E-07	-1.7137E-10	298	1200
33	C5H8O3	2-HYDROXYETHYL ACRYLATE	32.518	4.3890E-01	-2.5355E-04	6.9217E-08	-1.1605E-11	298	1500
34	C5H8O3	LEVULINIC ACID	-27.476	6.8761E-01	-6.6106E-04	3.5816E-07	-8.1625E-11	298	1500
35	C5H8O3	METHYL ACETOACETATE	2.795	7.1090E-01	-7.9710E-04	5.4496E-07	-1.6341E-10	298	1200
36	C5H8O4	GLUTARIC ACID	20.430	3.9187E-01	-1.7706E-04	1.0768E-08	9.2411E-12	200	1500
37	C5H9N	VALERONITRILE	25.162	3.1973E-01	3.5100E-05	-1.7032E-07	5.8493E-11	298	1100
38	C5H9NO	n-BUTYL ISOCYANATE	-46.964	5.6527E-01	-1.6330E-04	-1.9993E-07	1.2780E-10	298	1200
39	C5H9NO	N-METHYL-2-PYRROLIDONE	14.969	6.8061E-01	-5.5977E-04	2.4091E-07	-4.3844E-11	298	1500
40	C5H9NO4	L-GLUTAMIC ACID	19.735	1.1636E-01	5.1261E-04	-5.6745E-07	1.7045E-10	100	1500
41	C5H10	CYCLOPENTANE	36.231	2.5093E-01	8.9416E-05	-1.8917E-07	6.2160E-11	200	1500
42	C5H10	2-METHYL-1-BUTENE	39.489	1.9866E-01	1.8422E-04	-2.5432E-07	7.7912E-11	200	1500
43	C5H10	2-METHYL-2-BUTENE	34.280	3.1601E-01	-6.1287E-05	-6.6735E-08	2.8688E-11	200	1500
44	C5H10	3-METHYL-1-BUTENE	37.101	2.3664E-01	1.1834E-04	-2.1139E-07	6.8054E-11	200	1500
45	C5H10	1-PENTENE	24.729	2.5447E-01	1.1355E-04	-2.1629E-07	7.0502E-11	200	1500
46	C5H10	cis-2-PENTENE	38.859	2.2159E-01	1.3722E-04	-2.1992E-07	6.9261E-11	200	1500
47	C5H10	trans-2-PENTENE	4.347	5.8619E-01	-4.6054E-04	2.0428E-07	-3.9364E-11	298	1500
48	C5H10Cl2	1,5-DICHLOROPENTANE	-13.343	4.9441E-01	-2.5117E-04	2.5991E-08	9.7133E-12	298	1500
49	C5H10O	METHYL ISOPROPYL KETONE	42.356	2.7425E-01	6.3786E-05	-1.6870E-07	5.5342E-11	200	1500
50	C5H10O	2-PENTANONE	49.800	2.6897E-01	5.0669E-05	-1.5227E-07	4.9510E-11	200	1500
51	C5H10O	DIETHYL KETONE	26.913	3.5952E-01	-6.7847E-05	-7.0728E-08	2.9503E-11	273	1500
52	C5H10O	VALERALDEHYDE	-23.729	6.8205E-01	-6.0993E-04	3.0105E-07	-6.1033E-11	298	1500
53	C5H10O2	n-BUTYL FORMATE	139.382	-4.8565E-01	2.3071E-03	-2.7597E-06	1.0859E-09	298	1000
54	C5H10O2	ETHYL PROPIONATE	-26.232	6.8785E-01	-6.0138E-04	2.8357E-07	-5.3862E-11	298	1500
55	C5H10O2	ISOBUTYL FORMATE	-45.829	7.9654E-01	-7.9890E-04	4.3031E-07	-9.2988E-11	298	1500
56	C5H10O2	ISOPROPYL ACETATE	21.906	4.2733E-01	-1.3858E-04	-5.4238E-08	3.0118E-11	298	1500
57	C5H10O2	n-PROPYL ACETATE	-39.235	8.0965E-01	-9.2286E-04	6.0084E-07	-1.6118E-10	298	1200
58	C5H10O2	METHYL n-BUTYRATE	-19.156	6.0607E-01	-4.1921E-04	1.3696E-07	-1.7062E-11	298	1500
59	C5H10O2	2-METHYLBUTYRIC ACID	-5.803	5.9939E-01	-4.6602E-04	1.9713E-07	-3.6253E-11	298	1500
60	C5H10O2	ISOVALERIC ACID	-12.596	6.5474E-01	-5.8609E-04	2.8904E-07	-5.8646E-11	298	1500
61	C5H10O2	VALERIC ACID	-21.588	7.0118E-01	-6.2383E-04	3.0249E-07	-6.1395E-11	298	1500
62	C5H10O2	TETRAHYDROFURFURYL ALCOHOL							

$$C_p = A + B T + C T^2 + D T^3 + E T^4 \quad (C_p - \text{joule/g-mol K, } T - \text{K})$$

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
63	C5H10O2S	3-METHYL SULFOLANE	2.742	4.4985E-01	1.4128E-04	-4.9419E-07	2.1699E-10	298	1200
64	C5H10O3	DIETHYL CARBONATE	---	---	---	---	---	--	--
65	C5H10O3	ETHYL LACTATE	-30.734	8.0038E-01	-8.1025E-04	4.4743E-07	-9.9928E-11	298	1500
66	C5H11Cl	1-CHLOROPENTANE	22.357	4.1358E-01	-1.2716E-04	-4.7751E-08	2.7004E-11	200	1500
67	C5H11N	N-METHYLPYRROLIDINE	-63.618	6.8971E-01	-4.8249E-04	1.6504E-07	-2.1384E-11	298	1500
68	C5H11N	PIPERIDINE	-53.313	7.5541E-01	-5.6470E-04	1.6625E-07	-1.0457E-11	298	1500
69	C5H11NO	tert-BUTYLFORMAMIDE	-18.333	5.7294E-01	-2.9150E-04	-1.2192E-08	3.9907E-11	298	1200
70	C5H12	ISOPENTANE	-0.881	4.7498E-01	-2.4797E-04	6.7512E-08	-8.5343E-12	200	1500
71	C5H12	NEOPENTANE	-17.917	5.7236E-01	-4.1705E-04	2.1158E-07	-5.1006E-11	200	1500
72	C5H12	n-PENTANE	26.671	3.2324E-01	4.2820E-05	-1.6639E-07	5.6036E-11	200	1500
73	C5H12O	2,2-DIMETHYL-1-PROPANOL	-24.052	6.5427E-01	-4.7894E-04	1.6991E-07	-2.1290E-11	298	1500
74	C5H12O	2-METHYL-1-BUTANOL	-19.293	6.3101E-01	-4.7958E-04	1.9533E-07	-3.1575E-11	298	1500
75	C5H12O	2-METHYL-2-BUTANOL	-16.955	6.5298E-01	-5.4260E-04	2.6069E-07	-5.4462E-11	298	1200
76	C5H12O	3-METHYL-1-BUTANOL	17.380	3.8036E-01	9.0875E-05	-3.3684E-07	1.4257E-10	298	1200
77	C5H12O	3-METHYL-2-BUTANOL	-14.366	6.2608E-01	-4.8709E-04	2.1430E-07	-4.1705E-11	298	1500
78	C5H12O	1-PENTANOL	9.175	4.7662E-01	-1.9542E-04	-1.3991E-08	2.0685E-11	200	1500
79	C5H12O	2-PENTANOL	-7.077	5.9369E-01	-4.3971E-04	1.8499E-07	-3.5235E-11	298	1400
80	C5H12O	3-PENTANOL	61.233	7.9840E-02	9.0823E-04	-1.2984E-06	5.4866E-10	298	1000
81	C5H12O	METHYL sec-BUTYL ETHER	-0.104	5.5588E-01	-3.6662E-04	1.3167E-07	-2.0764E-11	298	1500
82	C5H12O	METHYL tert-BUTYL ETHER	39.585	2.8849E-01	1.3825E-04	-2.5131E-07	8.0807E-11	200	1500
83	C5H12O	METHYL ISOBUTYL ETHER	-11.287	5.9389E-01	-4.4085E-04	2.0554E-07	-4.9208E-11	298	1200
84	C5H12O	ETHYL PROPYL ETHER	14.457	4.5609E-01	-1.7751E-04	-1.1636E-08	1.6934E-11	298	1500
85	C5H12O2	ETHYLENE GLYCOL MONOPROPYL ETHER	-16.033	6.8258E-01	-5.7788E-04	2.9935E-07	-7.2869E-11	298	1200
86	C5H12O2	NEOPENTYL GLYCOL	-11.513	6.5964E-01	-4.8149E-04	1.8407E-07	-3.1786E-11	298	1500
87	C5H12O2	1,5-PENTANEDIOL	-2.425	6.1055E-01	-4.3769E-04	1.6872E-07	-2.6880E-11	298	1500
88	C5H12O3	2-(2-METHOXYETHOXY)ETHANOL	-22.744	7.9858E-01	-8.1464E-04	5.3038E-07	-1.5753E-10	298	1200
89	C5H12O4	PENTAERYTHRITOL	-4.675	7.5699E-01	-6.1689E-04	2.7195E-07	-5.3121E-11	298	1400
90	C5H12S	n-PENTYL MERCAPTAN	19.604	4.6839E-01	-2.0875E-04	4.3242E-08	-7.5836E-12	273	1500
91	C5H13N	n-PENTYLAMINE	6.603	5.2073E-01	-2.5708E-04	3.9765E-08	3.5264E-12	298	1500
92	C5H13NO2	METHYL DIETHANOLAMINE	-16.817	7.4349E-01	-5.5635E-04	2.1535E-07	-3.4622E-11	298	1500
93	C6Cl6	HEXACHLOROBENZENE	40.828	6.3403E-01	-7.3328E-04	4.0581E-07	-8.6866E-11	200	1500
94	C6F6	HEXAFLUOROBENZENE	56.398	4.1193E-01	-2.7480E-04	8.4094E-08	-7.9692E-12	200	1500
95	C6H3Cl2NO4	1-CHLORO-2,4-DINITROBENZENE	36.588	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
96	C6H3Cl2NO2	1,2-DICHLORO-4-NITROBENZENE	20.678	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
97	C6H3Cl3	1,2,4-TRICHLOROBENZENE	2.547	5.6873E-01	-5.5217E-04	2.6984E-07	-5.2816E-11	200	1500
98	C6H3N3O6	1,3,5-TRINITROBENZENE	52.498	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
99	C6H4Br2	m-DIBROMOBENZENE	23.494	3.7580E-01	-1.7947E-04	-1.2488E-08	2.2028E-11	150	1500
100	C6H4ClNO2	m-CHLORONITROBENZENE	2.238	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
101	C6H4ClNO2	o-CHLORONITROBENZENE	5.599	5.4506E-01	-3.6483E-04	8.1076E-08	3.5675E-12	200	1500
102	C6H4ClNO2	p-CHLORONITROBENZENE	2.861	5.6351E-01	-3.9804E-04	1.0486E-07	-2.4547E-12	200	1500
103	C6H4Cl2	m-DICHLOROBENZENE	-9.294	5.4269E-01	-4.8322E-04	2.1721E-07	-3.9293E-11	200	1500
104	C6H4Cl2	o-DICHLOROBENZENE	-9.539	5.4073E-01	-4.7821E-04	2.1330E-07	-3.8284E-11	200	1500
105	C6H4Cl2	p-DICHLOROBENZENE	-9.451	5.4233E-01	-4.8126E-04	2.1537E-07	-3.8775E-11	200	1500
106	C6H4N2O4	m-DINITROBENZENE	18.148	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
107	C6H4N2O4	o-DINITROBENZENE	18.148	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
108	C6H4N2O4	p-DINITROBENZENE	18.148	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
109	C6H5Br	BROMOBENZENE	10.965	3.3493E-01	-7.7630E-05	-9.0065E-08	4.1966E-11	200	1500
110	C6H5Cl	MONOCHLOROBENZENE	27.315	2.4405E-01	9.3748E-05	-2.2377E-07	8.0155E-11	200	1500
111	C6H5ClO	m-CHLOROPHENOL	-30.256	6.6657E-01	-6.5807E-04	3.2782E-07	-6.5085E-11	298	1500
112	C6H5ClO	o-CHLOROPHENOL	-30.256	6.6657E-01	-6.5807E-04	3.2782E-07	-6.5085E-11	298	1500
113	C6H5ClO	p-CHLOROPHENOL	-30.256	6.6657E-01	-6.5807E-04	3.2782E-07	-6.5085E-11	298	1500
114	C6H5Cl2N	3,4-DICHLOROANILINE	-12.710	6.9240E-01	-7.0094E-04	3.5781E-07	-7.2645E-11	298	1500
115	C6H5F	FLUOROBENZENE	-7.810	4.1311E-01	-1.9932E-04	-6.0575E-09	2.0763E-11	200	1500
116	C6H5I	IODOBENZENE	5.014	3.8494E-01	-1.7674E-04	-1.4239E-08	2.1809E-11	200	1500
117	C6H5NO2	NITROBENZENE	-16.202	5.6182E-01	-3.9302E-04	1.0043E-07	-1.2252E-12	200	1500
118	C6H6	BENZENE	-31.368	4.7460E-01	-3.1137E-04	8.5237E-08	-5.0524E-12	200	1500
119	C6H6ClN	m-CHLOROANILINE	-24.493	6.6130E-01	-6.1856E-04	2.9376E-07	-5.6020E-11	298	1500
120	C6H6ClN	o-CHLOROANILINE	-24.493	6.6130E-01	-6.1856E-04	2.9376E-07	-5.6020E-11	298	1500
121	C6H6ClN	p-CHLOROANILINE	-24.135	6.5666E-01	-6.0355E-04	2.7595E-07	-4.8992E-11	298	1200
122	C6H6N2	cis-DICYANO-1-BUTENE	6.870	4.1827E-01	-7.9183E-05	-2.1892E-07	1.2143E-10	298	1000
123	C6H6N2	trans-DICYANO-1-BUTENE	-1.571	5.5288E-01	-4.8007E-04	2.1814E-07	-4.0133E-11	298	1500
124	C6H6N2	1,4-DICYANO-2-BUTENE	39.740	2.7876E-01	1.3446E-04	-3.5716E-07	1.5299E-10	298	1000
125	C6H6N2O2	m-NITROANILINE	12.288	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500
126	C6H6N2O2	o-NITROANILINE	12.288	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500
127	C6H6N2O2	p-NITROANILINE	12.288	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500
128	C6H6O	PHENOL	4.408	3.6338E-01	-6.0417E-05	-1.2794E-07	5.5287E-11	100	1500
129	C6H6O2	1,2-BENZENEDIOL	-24.649	6.2268E-01	-5.0070E-04	1.8696E-07	-2.5672E-11	200	1500
130	C6H6O2	1,3-BENZENEDIOL	-28.476	6.8792E-01	-6.7225E-04	3.3593E-07	-6.7411E-11	200	1500
131	C6H6O2	p-HYDROQUINONE	-23.109	6.6077E-01	-6.4518E-04	3.2817E-07	-6.7604E-11	200	1500
132	C6H6O3	1,2,3-BENZENETRIOL	-23.381	7.5537E-01	-7.6515E-04	3.8498E-07	-7.6871E-11	298	1500
133	C6H6S	PHENYL MERCAPTAN	-5.259	4.4764E-01	-2.3973E-04	2.2703E-08	1.2746E-11	200	1500
134	C6H7N	ANILINE	-22.062	5.7313E-01	-4.5651E-04	1.8410E-07	-2.9867E-11	200	1500

			$C_p = A + B T + C T^2 + D T^3 + E T^4$ (C_p - joule/g-mol K, T - K)						
NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
135	C6H7N	2-METHYLPYRIDINE	-17.819	4.7591E-01	-2.5380E-04	3.3280E-08	8.7218E-12	200	1500
136	C6H7N	3-METHYLPYRIDINE	-16.136	4.6342E-01	-2.2923E-04	1.6537E-08	1.2749E-11	200	1500
137	C6H7N	4-METHYLPYRIDINE	-18.170	4.7450E-01	-2.4996E-04	3.0282E-08	9.4921E-12	200	1500
138	C6H8	1,3-CYCLOHEXADIENE	9.959	2.5557E-01	2.0432E-04	-3.3043E-07	1.0763E-10	100	1500
139	C6H8	METHYLCYCLOPENTADIENE	-59.926	7.1827E-01	-6.8011E-04	3.3399E-07	-6.6324E-11	298	1500
140	C6H8N2	ADIPONITRILE	46.703	2.1098E-01	6.0849E-04	-1.0564E-06	4.7126E-10	298	1000
141	C6H8N2	METHYLGUTARONITRILE	32.077	4.3754E-01	-2.3741E-04	4.6871E-08	4.8993E-13	298	1500
142	C6H8N2	m-PHENYLENEDIAMINE	-35.663	7.5211E-01	-7.0735E-04	3.3963E-07	-6.5853E-11	298	1500
143	C6H8N2	o-PHENYLENEDIAMINE	-35.663	7.5211E-01	-7.0735E-04	3.3963E-07	-6.5853E-11	298	1500
144	C6H8N2	p-PHENYLENEDIAMINE	-35.663	7.5211E-01	-7.0735E-04	3.3963E-07	-6.5853E-11	298	1500
145	C6H8N2	PHENYLHYDRAZINE	-53.505	7.8460E-01	-7.4455E-04	3.6656E-07	-7.3334E-11	298	1500
146	C6H8N2O	BIS(CYANOETHYL)ETHER	30.043	4.8287E-01	-2.4564E-04	1.9368E-08	1.2919E-11	298	1500
147	C6H8O4	DIMETHYL MALEATE	-1.849	7.6196E-01	-7.8473E-04	4.5797E-07	-1.1125E-10	298	1200
148	C6H8O6	ASCORBIC ACID	-7.357	1.0100E+00	-1.1580E-03	6.7650E-07	-1.5220E-10	298	1500
149	C6H8O7	CITRIC ACID	20.051	8.5219E-01	-8.1655E-04	4.0741E-07	-8.3420E-11	298	1500
150	C6H10	CYCLOHEXENE	11.332	2.5648E-01	2.9121E-04	-4.0917E-07	1.2869E-10	100	1500
151	C6H10	2,3-DIMETHYL-1,3-BUTADIENE	-14.346	6.3345E-01	-5.7820E-04	2.9473E-07	-6.2408E-11	298	1500
152	C6H10	1,5-HEXADIENE	-19.919	5.8801E-01	-4.6457E-04	2.0423E-07	-3.8563E-11	298	1500
153	C6H10	cis,trans-2,4-HEXADIENE	-21.887	5.8531E-01	-4.4663E-04	1.8361E-07	-3.2586E-11	298	1500
154	C6H10	trans,trans-2,4-HEXADIENE	-13.866	5.8123E-01	-4.6720E-04	2.1027E-07	-4.0509E-11	298	1500
155	C6H10	1-HEXYNE	19.611	4.4045E-01	-2.3708E-04	4.1265E-08	3.5316E-12	200	1500
156	C6H10	2-HEXYNE	-3.658	5.1409E-01	-3.7142E-04	1.5649E-07	-2.7818E-11	298	1500
157	C6H10	3-HEXYNE	-12.209	5.5220E-01	-4.4735E-04	2.2254E-07	-4.7781E-11	298	1500
158	C6H10O	CYCLOHEXANONE	-12.337	4.0837E-01	1.0597E-04	-2.9616E-07	1.0088E-10	200	1500
159	C6H10O	MESITYL OXIDE	16.062	5.8779E-01	-6.0312E-04	4.4456E-07	-1.4943E-10	298	1000
160	C6H10O2	epsilon-CAPROLACTONE	-59.878	7.3431E-01	-4.4185E-04	9.0409E-08	3.2030E-12	298	1500
161	C6H10O2	ETHYL METHACRYLATE	-38.063	7.5789E-01	-6.5982E-04	3.0689E-07	-5.9646E-11	298	1500
162	C6H10O2	n-PROPYL ACRYLATE	-34.027	8.8100E-01	-9.6426E-04	5.6512E-07	-1.2909E-10	298	1500
163	C6H10O3	ETHYLACETOACETATE	-38.431	8.1942E-01	-7.5317E-04	3.7707E-07	-7.8132E-11	298	1500
164	C6H10O3	PROPIONIC ANHYDRIDE	29.000	3.6844E-01	3.0361E-04	-6.2082E-07	2.4092E-10	298	1200
165	C6H10O4	ADIPIC ACID	7.418	6.7710E-01	-4.6904E-04	1.4619E-07	-1.5583E-11	298	1500
166	C6H10O4	DIETHYL OXALATE	-63.195	1.0643E+00	-1.1909E-03	6.9357E-07	-1.5592E-10	298	1500
167	C6H10O4	ETHYLENE GLYCOL DIACETATE	-63.207	1.0644E+00	-1.1911E-03	6.9374E-07	-1.5597E-10	298	1500
168	C6H10O4	ETHYLIDENE DIACETATE	-11.375	5.4896E-01	3.3144E-04	-1.0756E-06	5.5152E-10	298	1000
169	C6H11N	HEXANENITRILE	23.213	4.6598E-01	-1.9041E-04	-8.6856E-09	1.7539E-11	200	1500
170	C6H11NO	epsilon-CAPROLACTAM	-10.914	2.7864E-01	6.5610E-04	-9.5916E-07	3.6689E-10	298	1000
171	C6H11NO	CYCLOHEXANONE OXIME	-38.514	6.5385E-01	-2.3559E-04	7.2552E-08	4.5887E-11	298	1500
172	C6H12	CYCLOHEXANE	13.783	2.0742E-01	5.3682E-04	-6.3012E-07	1.8988E-10	100	1500
173	C6H12	2,3-DIMETHYL-1-BUTENE	32.307	4.2869E-01	-1.5601E-04	-2.1440E-08	1.8781E-11	200	1500
174	C6H12	2,3-DIMETHYL-2-BUTENE	50.138	1.9488E-01	3.1558E-04	-3.7082E-07	1.0920E-10	200	1500
175	C6H12	3,3-DIMETHYL-1-BUTENE	37.579	2.8542E-01	1.8034E-04	-3.0375E-07	9.8601E-11	200	1500
176	C6H12	2-ETHYL-1-BUTENE	26.884	3.9566E-01	-5.3867E-05	-1.1252E-07	4.5467E-11	200	1500
177	C6H12	1-HEXENE	32.517	3.5231E-01	2.2971E-05	-1.6592E-07	5.8510E-11	200	1500
178	C6H12	cis-2-HEXENE	35.642	2.9178E-01	1.5778E-04	-2.7413E-07	8.8092E-11	200	1500
179	C6H12	trans-2-HEXENE	49.211	2.6046E-01	1.8185E-04	-2.8038E-07	8.7781E-11	200	1500
180	C6H12	cis-3-HEXENE	58.647	1.3967E-01	4.7553E-04	-5.3528E-07	1.6155E-10	150	1500
181	C6H12	trans-3-HEXENE	66.499	1.6110E-01	3.8543E-04	-4.4785E-07	1.3530E-10	150	1500
182	C6H12	METHYLCYCLOPENTANE	-9.939	4.2528E-01	1.2521E-05	-1.8864E-07	6.4751E-11	200	1500
183	C6H12	2-METHYL-1-PENTENE	35.161	3.5515E-01	1.6698E-05	-1.6387E-07	5.7999E-11	200	1500
184	C6H12	2-METHYL-2-PENTENE	27.059	3.4858E-01	4.7035E-05	-1.9000E-07	6.5743E-11	200	1500
185	C6H12	3-METHYL-1-PENTENE	59.573	2.5875E-01	1.8945E-04	-3.0001E-07	9.6074E-11	150	1500
186	C6H12	3-METHYL-cis-2-PENTENE	58.069	1.6574E-01	4.0178E-04	-4.6769E-07	1.4145E-10	150	1500
187	C6H12	4-METHYL-1-PENTENE	26.362	3.5120E-01	3.9961E-05	-1.8537E-07	6.4392E-11	200	1500
188	C6H12	4-METHYL-cis-2-PENTENE	52.969	2.5164E-01	2.0116E-04	-3.0068E-07	9.5720E-11	200	1500
189	C6H12	4-METHYL-trans-2-PENTENE	39.751	3.7243E-01	-5.1165E-05	-9.8996E-08	3.8818E-11	200	1500
190	C6H12N2	TRIETHYLENEDIAMINE	-124.418	1.0337E+00	-8.2395E-04	3.2203E-07	-4.8974E-11	298	1500
191	C6H12O	BUTYL VINYL ETHER	-1.119	5.8419E-01	-3.7075E-04	1.2882E-07	-2.3385E-11	298	1500
192	C6H12O	CYCLOHEXANOL	17.124	3.3700E-01	2.8176E-04	-4.2713E-07	1.3215E-10	200	1500
193	C6H12O	1-HEXANAL	71.773	2.0294E-01	3.4761E-04	-4.1609E-07	1.2259E-10	200	1500
194	C6H12O	ETHYL ISOPROPYL KETONE	36.515	3.4267E-01	1.4830E-04	-3.4209E-07	1.3148E-10	298	1200
195	C6H12O	2-HEXANONE	45.050	3.5513E-01	4.8896E-05	-1.9813E-07	6.4005E-11	200	1500
196	C6H12O	3-HEXANONE	73.031	2.2148E-01	2.7912E-04	-3.6876E-07	1.1286E-10	150	1500
197	C6H12O	METHYL ISOBUTYL KETONE	2.404	5.8495E-01	-3.7647E-04	1.2418E-07	-1.7051E-11	298	1500
198	C6H12O2	n-PENTYL FORMATE	-30.624	8.1555E-01	-7.4226E-04	3.7578E-07	-7.8511E-11	298	1500
199	C6H12O2	n-BUTYL ACETATE	85.139	7.1561E-02	8.7842E-04	-1.0725E-06	3.7362E-10	298	1200
200	C6H12O2	sec-BUTYL ACETATE	-37.391	8.3030E-01	-6.9627E-04	2.6603E-07	-2.1215E-11	298	1000
201	C6H12O2	tert-BUTYL ACETATE	-66.418	1.0291E+00	-1.1512E-03	7.0828E-07	-1.7774E-10	298	1200
202	C6H12O2	ETHYL n-BUTYRATE	-16.529	7.2624E-01	-5.1890E-04	1.2305E-07	2.3936E-11	298	1200
203	C6H12O2	ETHYL ISOBUTYRATE	-62.802	9.3400E-01	-9.1286E-04	4.8405E-07	-1.0440E-10	298	1500
204	C6H12O2	ISOBUTYL ACETATE	-24.628	7.5868E-01	-5.9783E-04	2.3506E-07	-3.4297E-11	298	1500
205	C6H12O2	n-PROPYL PROPIONATE	-26.162	7.8326E-01	-6.3633E-04	2.2535E-07	-8.0808E-12	298	1200
206	C6H12O2	CYCLOHEXYL PEROXIDE	-66.681	9.6297E-01	-1.0232E-03	7.4423E-07	-2.5645E-10	298	1000

NO	FORMULA	NAME	$C_p = A + B T + C T^2 + D T^3 + E T^4$					$(C_p - \text{joule/g-mol K, } T - K)$	
			A	B	C	D	E	TMIN	TMAX
207	C6H12O2	DIACETONE ALCOHOL	13.030	5.9591E-01	-3.8411E-04	1.5153E-07	-3.8398E-11	298	1200
208	C6H12O2	2-ETHYL BUTYRIC ACID	-44.341	8.5885E-01	-8.2522E-04	4.6805E-07	-1.1743E-10	298	1200
209	C6H12O2	n-HEXANOIC ACID	-9.559	7.4029E-01	-6.6784E-04	3.7713E-07	-1.0030E-10	298	1200
210	C6H12O3	2-ETHOXYETHYL ACETATE	-34.381	8.6550E-01	-7.7015E-04	3.7720E-07	-8.0618E-11	298	1500
211	C6H12O3	HYDROXYCAPROIC ACID	-2.103	7.3513E-01	-5.5705E-04	2.2007E-07	-3.6780E-11	298	1500
212	C6H12O3	PARALDEHYDE	-129.363	1.2890E+00	-1.4032E-03	7.4424E-07	-1.4315E-10	298	1500
213	C6H12O3	sec-BUTYL GLYCOLATE	---	---	---	---	---	---	---
214	C6H13N	CYCLOHEXYLAMINE	-47.225	7.0490E-01	-3.4142E-04	1.8298E-08	1.9665E-11	298	1500
215	C6H13N	HEXAMETHYLENEIMINE	-81.362	7.9390E-01	-4.5964E-04	9.4512E-08	2.5824E-12	298	1400
216	C6H14	2,2-DIMETHYLBUTANE	-1.477	5.5644E-01	-2.4802E-04	4.1433E-08	2.4035E-13	200	1500
217	C6H14	2,3-DIMETHYLBUTANE	-25.999	6.8344E-01	-4.8517E-04	2.1262E-07	-4.3837E-11	200	1500
218	C6H14	n-HEXANE	25.924	4.1927E-01	-1.2491E-05	-1.5916E-07	5.8784E-11	200	1500
219	C6H14	2-METHYLPENTANE	-7.197	6.0097E-01	-3.4094E-04	9.5210E-08	-1.0297E-11	200	1500
220	C6H14	3-METHYLPENTANE	-7.123	5.8327E-01	-3.0338E-04	6.8016E-08	-3.9778E-12	200	1500
221	C6H14N2O2	LYSINE	3.524	8.1910E-01	-6.3474E-04	2.7688E-07	-5.6094E-11	298	1500
222	C6H14O	2-ETHYL-1-BUTANOL	-25.284	7.6092E-01	-6.1315E-04	2.7815E-07	-5.3099E-11	298	1500
223	C6H14O	1-HEXANOL	10.719	5.5767E-01	-2.1818E-04	-3.2298E-08	2.9769E-11	200	1500
224	C6H14O	2-HEXANOL	-8.756	6.7929E-01	-4.4926E-04	1.4008E-07	-1.1453E-11	298	1200
225	C6H14O	2-METHYL-1-PENTANOL	-18.096	7.1113E-01	-5.2110E-04	2.1617E-07	-4.0923E-11	298	1500
226	C6H14O	4-METHYL-2-PENTANOL	-17.282	7.3333E-01	-5.6666E-04	2.4735E-07	-4.7894E-11	298	1500
227	C6H14O	n-BUTYL ETHYL ETHER	10.663	5.7291E-01	-2.7890E-04	3.8539E-08	6.0989E-12	298	1500
228	C6H14O	DIISOPROPYL ETHER	92.068	1.1054E-01	5.8784E-04	-6.1854E-07	1.7855E-10	100	1500
229	C6H14O	DI-n-PROPYL ETHER	-26.082	7.6707E-01	-6.4734E-04	3.3945E-07	-8.3996E-11	298	1200
230	C6H14O	METHYL tert-PENTYL ETHER	-5.816	6.8044E-01	-4.6708E-04	1.7397E-07	-2.8573E-11	298	1500
231	C6H14O2	ACETAL	31.834	3.4539E-01	5.6817E-04	-1.0268E-06	4.4628E-10	298	1000
232	C6H14O2	2-BUTOXYETHANOL	-22.219	8.1143E-01	-7.1242E-04	3.9347E-07	-1.0334E-10	298	1200
233	C6H14O2	1,6-HEXANEDIOL	-2.789	7.0351E-01	-4.9185E-04	1.8516E-07	-3.0221E-11	298	1500
234	C6H14O2	HEXYLENE GLYCOL	-30.746	8.8908E-01	-8.0455E-04	4.0021E-07	-8.2866E-11	298	1500
235	C6H14O2S	DI-n-PROPYL SULFONE	16.469	6.7237E-01	-3.3664E-04	5.5367E-08	4.0249E-12	298	1500
236	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER	-38.307	9.9161E-01	-1.1006E-03	7.7626E-07	-2.4078E-10	298	1200
237	C6H14O3	DIPROPYLENE GLYCOL	-31.988	9.4839E-01	-8.9835E-04	4.8010E-07	-1.1001E-10	298	1200
238	C6H14O3	2-(2-ETHOXYETHOXY)ETHANOL	-15.223	8.0630E-01	-6.0939E-04	2.4852E-07	-4.4531E-11	298	1500
239	C6H14O3	TRIMETHYLOLPROPANE	-14.530	8.3299E-01	-6.6014E-04	2.7694E-07	-4.8128E-11	298	1500
240	C6H14O4	TRIMETHYLENE GLYCOL	2.101	7.8650E-01	-5.6060E-04	2.0905E-07	-3.3896E-11	298	1500
241	C6H14O6	SORBITOL	-6.695	1.0042E+00	-7.9252E-04	2.0507E-07	3.0979E-11	298	1200
242	C6H14S	n-HEXYLMERCAPTAN	56.097	3.5459E-01	1.3831E-04	-2.6776E-07	8.5007E-11	200	1500
243	C6H15Al	TRIETHYL ALUMINUM	---	---	---	---	---	---	---
244	C6H15Al2Cl3	3ETHYL ALUMINUM SESQUICHLORIDE	123.889	2.1683E-01	6.9390E-04	-8.2388E-07	2.5547E-10	100	1500
245	C6H15N	DIISOPROPYLAMINE	-38.690	8.3934E-01	-6.8079E-04	3.1403E-07	-6.5038E-11	298	1500
246	C6H15N	DI-n-PROPYLAMINE	-35.272	8.1873E-01	-6.6672E-04	3.1414E-07	-6.4824E-11	298	1500
247	C6H15N	n-HEXYLAMINE	62.901	3.0756E-01	2.3918E-04	-3.4644E-07	1.0365E-10	200	1500
248	C6H15N	TRIETHYLAMINE	55.793	3.3337E-01	2.2077E-04	-3.4942E-07	1.0838E-10	200	1500
249	C6H15NO	6-AMINOHEXANOL	10.049	6.6024E-01	-3.7498E-04	9.7671E-08	-1.2128E-11	298	1500
250	C6H15NO2	DIISOPROPANOLAMINE	-32.670	9.6179E-01	-8.5944E-04	4.1808E-07	-8.2801E-11	298	1200
251	C6H15NO3	TRITHANOLAMINE	37.730	4.9155E-01	3.5952E-04	-8.2287E-07	3.5374E-10	298	1200
252	C6H15N3	N-AMINOETHYL PIPERAZINE	-18.325	7.9527E-01	-4.9153E-04	1.3652E-07	-1.2092E-11	298	1500
253	C6H15O4P	TRIETHYL PHOSPHATE	---	---	---	---	---	---	---
254	C6H16N2	HEXAMETHYLENEDIAMINE	8.511	7.1350E-01	-4.7390E-04	2.1163E-07	-6.1825E-11	298	1200
255	C6H18N3OP	HEXAMETHYL PHOSPHORAMIDE	---	---	---	---	---	---	---
256	C6H18N4	TRIETHYLENE TETRAMINE	-26.003	1.0161E+00	-8.1609E-04	3.6628E-07	-7.0398E-11	298	1500
257	C6H18OSi2	HEXAMETHYLDISILOXANE	96.759	5.3023E-01	-1.0701E-04	-1.0135E-07	4.3962E-11	200	1500
258	C6H18O3Si3	HEXAMETHYLCYCLOTRISILOXANE	42.372	7.1830E-01	-3.5419E-05	-3.1816E-07	1.2408E-10	100	1500
259	C6H19NSi2	HEXAMETHYLDISILAZANE	-10.219	8.5172E-01	-4.3504E-04	6.1843E-08	9.4823E-12	298	1500
260	C7H3ClF3NO24	4-CHLORO-3-NITROBENZOTRIFLUORIDE	2.462	8.0944E-01	-8.0238E-04	3.9826E-07	-7.8100E-11	298	1600
261	C7H3Cl2F3	2,4-DICHLOROBENZOTRIFLUORIDE	-18.588	8.4436E-01	-8.9784E-04	4.7892E-07	-1.0373E-10	298	1200
262	C7H3Cl2NO	3,4-DICHLOROPHENYL ISOCYANATE	-88.252	1.2181E+00	-1.8543E-03	1.3889E-06	-3.9144E-10	298	1200
263	C7H4ClF3	p-CHLOROBENZOTRIFLUORIDE	-32.088	8.0944E-01	-8.0238E-04	3.9826E-07	-7.8100E-11	298	1600
264	C7H4Cl2O	m-CHLOROBENZOYL CHLORIDE	3.438	5.7712E-01	-4.8258E-04	2.0062E-07	-3.3551E-11	298	1500
265	C7H4F3NO2	3-NITROBENZOTRIFLUORIDE	-16.178	8.0944E-01	-8.0238E-04	3.9826E-07	-7.8100E-11	298	1600
266	C7H5ClO	BENZOYL CHLORIDE	-8.923	5.4527E-01	-4.0749E-04	1.4722E-07	-2.0723E-11	298	1500
267	C7H5ClO2	o-CHLOROBENZOIC ACID	8.444	3.3784E-01	3.0050E-04	-6.8672E-07	3.0928E-10	298	1000
268	C7H5Cl3	BENZOTRICHLORIDE	-17.223	7.3674E-01	-7.4806E-04	4.2367E-07	-1.0609E-10	298	1200
269	C7H5F3	BENZOTRIFLUORIDE	-5.571	5.6388E-01	-3.3437E-04	5.2123E-08	1.1313E-11	200	1500
270	C7H5N	BENZONITRILE	-2.624	4.5843E-01	-2.6757E-04	4.3711E-08	7.3182E-12	200	1500
271	C7H5NO	PHENYL ISOCYANATE	-28.586	5.8118E-01	-4.2739E-04	1.4817E-07	-1.9292E-11	298	1500
272	C7H5N3O6	2,4,6-TRINITROTOLUENE	78.953	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
273	C7H6Cl2	BENZYL DICHLORIDE	-23.635	6.5729E-01	-5.5210E-04	2.3709E-07	-4.1699E-11	298	1500
274	C7H6Cl2	2,4-DICHLOROTOLUENE	37.983	2.1821E-01	7.2356E-04	-1.2976E-06	6.0155E-10	298	1000
275	C7H6N2O4	2,4-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
276	C7H6N2O4	2,5-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
277	C7H6N2O4	2,6-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
278	C7H6N2O4	3,4-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500

$$C_p = A + B T + C T^2 + D T^3 + E T^4 \quad (C_p - \text{joule/g-mol K, } T - \text{K})$$

NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
279	C7H6N2O4	3,5-DINITROTOLUENE	44.603	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
280	C7H6O	BENZALDEHYDE	-0.890	4.4758E-01	-1.8566E-04	-3.6205E-08	3.1110E-11	200	1500
281	C7H6O2	BENZOIC ACID	16.158	2.8234E-01	1.7811E-04	-3.2176E-07	1.0752E-10	200	1500
282	C7H6O2	p-HYDROXYBENZALDEHYDE	-17.327	6.1293E-01	-3.6141E-04	4.2615E-08	1.8399E-11	298	1200
283	C7H6O2	SALICYLALDEHYDE	-33.117	7.0148E-01	-5.4741E-04	2.0112E-07	-2.8014E-11	298	1500
284	C7H6O3	SALICYLIC ACID	-4.230	5.4660E-01	-2.2561E-04	-5.4965E-07	2.6161E-10	298	1000
285	C7H7Br	p-BROMOTOLUENE	-11.148	5.5111E-01	-3.6702E-04	1.0465E-07	-8.5052E-12	298	1500
286	C7H7Cl	BENZYL CHLORIDE	-20.027	5.0561E-01	-3.9247E-04	1.4825E-07	-2.1517E-11	200	1500
287	C7H7Cl	o-CHLOROTOLUENE	-19.597	5.4660E-01	-2.2561E-04	-1.3546E-07	1.0757E-10	298	1000
288	C7H7Cl	p-CHLOROTOLUENE	-19.597	5.4660E-01	-2.2561E-04	-1.3546E-07	1.0757E-10	298	1000
289	C7H7NO	FORMANILIDE	-58.019	7.4752E-01	-6.4061E-04	2.6844E-07	-4.4253E-11	298	1500
290	C7H7NO2	m-NITROTOLUENE	10.253	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
291	C7H7NO2	o-NITROTOLUENE	10.253	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
292	C7H7NO2	p-NITROTOLUENE	10.253	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
293	C7H7NO3	o-NITROANISOLE	-11.742	6.4927E-01	-4.3634E-04	1.1823E-07	-3.1868E-12	298	1200
294	C7H8	TOLUENE	-24.097	5.2187E-01	-2.9827E-04	6.1220E-08	1.2576E-12	200	1500
295	C7H8O	ANISOLE	-46.092	6.4927E-01	-4.3634E-04	1.1823E-07	-3.1868E-12	298	1200
296	C7H8O	BENZYL ALCOHOL	-38.244	5.7295E-01	-1.9618E-04	-1.7885E-07	1.2218E-10	298	1000
297	C7H8O	m-CRESOL	-28.118	6.6639E-01	-5.5684E-04	2.4989E-07	-4.7599E-11	200	1500
298	C7H8O	o-CRESOL	-10.489	5.7475E-01	-3.8585E-04	1.1736E-07	-1.1385E-11	200	1500
299	C7H8O	p-CRESOL	-21.163	6.2005E-01	-4.6259E-04	1.7288E-07	-2.5755E-11	200	1500
300	C7H8O2	GUAIACOL	-53.237	8.0557E-01	-7.1471E-04	3.1975E-07	-5.4471E-11	298	1200
301	C7H8O2	p-METHOXYPHENOL	-55.124	8.2278E-01	-7.6384E-04	3.7503E-07	-7.5815E-11	298	1500
302	C7H9N	BENZYLAMINE	-44.632	7.3792E-01	-6.4144E-04	3.0305E-07	-6.0296E-11	298	1500
303	C7H9N	2,6-DIMETHYLPYRIDINE	-12.959	5.3389E-01	-2.5211E-04	1.2256E-08	1.5481E-11	200	1500
304	C7H9N	N-METHYLANILINE	-63.167	8.2599E-01	-7.5180E-04	3.5552E-07	-6.8719E-11	298	1500
305	C7H9N	m-TOLUIDINE	-15.216	5.9535E-01	-3.8755E-04	1.1831E-07	-1.2703E-11	200	1500
306	C7H9N	o-TOLUIDINE	-15.391	6.2396E-01	-4.3867E-04	1.5449E-07	-2.1698E-11	200	1500
307	C7H9N	p-TOLUIDINE	-18.360	6.1016E-01	-4.1260E-04	1.3537E-07	-1.6747E-11	200	1500
308	C7H10	2-NORBORNENE	-75.556	7.5963E-01	-5.2049E-04	1.6449E-07	-1.7953E-11	298	1500
309	C7H10N2	TOLUENEDIAMINE	-75.447	1.0663E+00	-1.1548E-03	6.1040E-07	-1.1054E-10	298	1500
310	C7H11NO	CYCLOHEXYL ISOCYANATE	-20.869	5.1917E-01	4.6475E-05	-2.9175E-07	1.0386E-10	298	1500
311	C7H12O2	n-BUTYL ACRYLATE	31.423	6.2124E-01	-3.6990E-04	1.0373E-07	-1.7445E-11	298	1000
312	C7H12O2	ISOBUTYL ACRYLATE	-39.964	9.9799E-01	-1.0514E-03	5.9928E-07	-1.3516E-10	298	1500
313	C7H12O2	n-PROPYL METHACRYLATE	-43.005	8.7703E-01	-7.6204E-04	3.5635E-07	-6.9619E-11	298	1500
314	C7H12O4	DIETHYL MALONATE	-85.174	1.2290E+00	-1.3284E-03	7.4897E-07	-1.6575E-10	298	1500
315	C7H14	CYCLOHEPTANE	9.447	3.5261E-01	3.7699E-04	-5.3869E-07	1.6956E-10	100	1500
316	C7H14	1,1-DIMETHYLCYCLOPENTANE	9.329	4.1173E-01	1.8706E-04	-3.7024E-07	1.2310E-10	200	1500
317	C7H14	cis-1,2-DIMETHYLCYCLOPENTANE	10.096	4.1584E-01	1.6872E-04	-3.5294E-07	1.1818E-10	200	1500
318	C7H14	trans-1,2-DIMETHYLCYCLOPENTANE	11.514	4.1203E-01	1.7044E-04	-3.5275E-07	1.1806E-10	200	1500
319	C7H14	cis-1,3-DIMETHYLCYCLOPENTANE	11.486	4.1227E-01	1.6993E-04	-3.5235E-07	1.1795E-10	200	1500
320	C7H14	trans-1,3-DIMETHYLCYCLOPENTANE	11.486	4.1227E-01	1.6993E-04	-3.5235E-07	1.1795E-10	200	1500
321	C7H14	ETHYLCYCLOPENTANE	-28.514	5.7607E-01	-9.4379E-05	-1.6445E-07	6.9435E-11	100	1500
322	C7H14	2-ETHYL-1-PENTENE	7.553	5.924E-01	-1.9092E-04	-5.9654E-08	3.5819E-11	298	1500
323	C7H14	3-ETHYL-1-PENTENE	2.696	5.6924E-01	-1.9489E-04	-6.2627E-08	3.7450E-11	298	1500
324	C7H14	1-HEPTENE	40.754	3.9922E-01	5.3848E-05	-2.1599E-07	7.4482E-11	200	1500
325	C7H14	cis-2-HEPTENE	-7.099	5.9005E-01	-2.3765E-04	-2.1795E-08	2.4907E-11	200	1500
326	C7H14	trans-2-HEPTENE	22.872	4.6064E-01	-1.9919E-05	-1.7969E-07	6.6169E-11	150	1500
327	C7H14	cis-3-HEPTENE	-25.417	6.7669E-01	-3.7697E-04	7.3028E-08	1.3960E-12	200	1500
328	C7H14	trans-3-HEPTENE	1.557	5.6602E-01	-1.9660E-04	-5.5257E-08	3.4487E-11	150	1500
329	C7H14	METHYLCYCLOHEXANE	4.296	4.2716E-01	2.1058E-04	-3.9987E-07	1.3121E-10	200	1500
330	C7H14	2-METHYL-1-HEXENE	13.419	5.3960E-01	-1.7371E-04	-6.3050E-08	3.5189E-11	298	1500
331	C7H14	3-METHYL-1-HEXENE	2.696	5.6924E-01	-1.9489E-04	-6.2627E-08	3.7450E-11	298	1500
332	C7H14	4-METHYL-1-HEXENE	-21.774	7.0339E-01	-4.4459E-04	1.2769E-07	-1.3424E-11	150	1500
333	C7H14	2,3,3-TRIMETHYL-1-BUTENE	0.695	6.0287E-01	-2.3415E-04	-4.8958E-08	3.6689E-11	298	1500
334	C7H14O	DIISOPROPYL KETONE	-59.457	8.9163E-01	-7.3368E-04	3.3507E-07	-6.4643E-11	298	1500
335	C7H14O	2-HEPTANONE	77.352	2.5365E-01	3.8252E-04	-4.9648E-07	1.4916E-10	150	1500
336	C7H14O	1-HEPTANAL	76.088	2.6868E-01	3.5354E-04	-4.5649E-07	1.3757E-10	200	1500
337	C7H14O	1-METHYLCYCLOHEXANOL	-54.565	8.4577E-01	-5.7323E-04	2.3275E-07	-5.9702E-11	298	1200
338	C7H14O	cis-2-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
339	C7H14O	trans-2-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
340	C7H14O	cis-3-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
341	C7H14O	trans-3-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
342	C7H14O	cis-4-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
343	C7H14O	trans-4-METHYLCYCLOHEXANOL	-47.283	7.6999E-01	-3.7628E-04	3.6819E-08	7.7738E-12	298	1200
344	C7H14O	5-METHYL-2-HEXANONE	-3.763	7.0117E-01	-4.7468E-04	1.8106E-07	-3.3882E-11	298	1200
345	C7H14O2	n-BUTYL PROPIONATE	-3.593	7.7324E-01	-5.9004E-04	2.9563E-07	-8.6992E-11	298	1200
346	C7H14O2	ETHYL ISOVALERATE	-45.699	9.9698E-01	-9.7130E-04	5.3585E-07	-1.2593E-10	298	1200
347	C7H14O2	ISOPENTYL ACETATE	-51.790	9.8897E-01	-9.0976E-04	4.6383E-07	-1.0053E-10	298	1500
348	C7H14O2	n-PENTYL ACETATE	-31.967	8.9188E-01	-7.5408E-04	3.6684E-07	-8.2457E-11	298	1200
349	C7H14O2	n-PROPYL n-BUTYRATE	-8.783	8.0270E-01	-6.4913E-04	3.4629E-07	-1.0270E-10	298	1200
350	C7H14O2	n-HEPTANOIC ACID	11.779	6.9196E-01	-4.1039E-04	1.1266E-07	-1.5295E-11	298	1500

			$C_p = A + B T + C T^2 + D T^3 + E T^4$					(C _p - joule/g-mol K, T - K)	
NO	FORMULA	NAME	A	B	C	D	E	TMIN	TMAX
351	C7H14O3	ETHYL-3-ETHOXYPROPIONATE	-62.701	1.1653E+00	-1.2886E-03	8.0077E-07	-2.0569E-10	298	1200
352	C7H15Br	1-BROMOHEPTANE	-11.271	7.7970E-01	-5.4848E-04	1.9542E-07	-2.5440E-11	298	1200
353	C7H15N	N-METHYLCYCLOHEXYLAMINE	-59.516	8.3575E-01	-4.3148E-04	4.6928E-08	1.6571E-11	298	1500
354	C7H16	2,2-DIMETHYLPENTANE	-19.277	7.6888E-01	-5.1678E-04	2.0476E-07	-3.7168E-11	200	1500
355	C7H16	2,3-DIMETHYLPENTANE	38.654	3.7259E-01	2.7632E-04	-4.3148E-07	1.3811E-10	100	1500
356	C7H16	2,4-DIMETHYLPENTANE	-32.996	8.7352E-01	-7.3286E-04	3.6633E-07	-7.9787E-11	200	1500
357	C7H16	3,3-DIMETHYLPENTANE	-23.909	7.8329E-01	-5.3992E-04	2.2604E-07	-4.4324E-11	200	1500
358	C7H16	3-ETHYLPENTANE	19.245	5.5072E-01	-1.4055E-04	-8.2482E-08	3.9487E-11	200	1500
359	C7H16	n-HEPTANE	26.984	5.0387E-01	-4.4748E-05	-1.6835E-07	6.5183E-11	200	1500
360	C7H16	2-METHYLHEXANE	-3.249	6.6625E-01	-3.3836E-04	6.0489E-08	2.5385E-12	200	1500
361	C7H16	3-METHYLHEXANE	-12.841	7.1358E-01	-4.2021E-04	1.1997E-07	-1.2906E-11	200	1500
362	C7H16	2,2,3-TRIMETHYLBUTANE	-21.150	7.4663E-01	-4.6699E-04	1.7923E-07	-3.4265E-11	200	1500
363	C7H16O	1-HEPTANOL	11.810	6.4236E-01	-2.4939E-04	-4.3649E-08	3.7035E-11	200	1500
364	C7H16O	2-HEPTANOL	-28.784	8.8407E-01	-7.1442E-04	3.2639E-07	-6.5218E-11	298	1500
365	C7H16O	5-METHYL-1-HEXANOL	0.274	6.8732E-01	-3.1154E-04	-1.1838E-08	3.5683E-11	298	1200
366	C7H16S	n-HEPTYL MERCAPTAN	59.314	4.3814E-01	8.8964E-05	-2.6174E-07	8.7398E-11	200	1500
367	C7H17N	1-AMINOHEPTANE	-1.435	7.4857E-01	-4.4543E-04	1.3200E-07	-1.8684E-11	298	1500

Appendix F

COMPOUND LIST BY FORMULA

CBrc1f2	BROMOCHLORODIFLUOROMETHANE.....	1(Vol 1)	C2H2Cl20	CHLOROACETYL CHLORIDE.....	71(Vol 1)
CBrc13	BROMOTRICHLOROMETHANE.....	2(Vol 1)	C2H2Cl20	DICHLOROACETALDEHYDE.....	72(Vol 1)
CBrcF3	BROMOTRIFLUOROMETHANE.....	3(Vol 1)	C2H2Cl202	DICHLOROACETIC ACID.....	73(Vol 1)
CBrc2F2	DIBROMODIFLUOROMETHANE.....	4(Vol 1)	C2H2Cl3F	1,1,1-TRICHLOROFLUOROETHANE.....	74(Vol 1)
CClF3	CHLOROTRIFLUOROMETHANE.....	5(Vol 1)	C2H2Cl4	1,1,1,2-TETRACHLOROETHANE.....	75(Vol 1)
CClN	CYANOGEN CHLORIDE.....	6(Vol 1)	C2H2Cl4	1,1,2,2-TETRACHLOROETHANE.....	76(Vol 1)
CCl2F2	DICHLORODIFLUOROMETHANE.....	7(Vol 1)	C2H2F2	1,1-DIFLUOROETHYLENE.....	77(Vol 1)
CCl2O	PHOSGENE.....	8(Vol 1)	C2H2F4	1,1,1,2-TETRAFLUOROETHANE.....	78(Vol 1)
CCl3F	TRICHLOROFLUOROMETHANE.....	9(Vol 1)	C2H2O	KETENE.....	79(Vol 1)
CCl4	CARBON TETRACHLORIDE.....	10(Vol 1)	C2H2O4	OXALIC ACID.....	80(Vol 1)
CF2O	CARBONYL FLUORIDE.....	11(Vol 1)	C2H3Br	VINYL BROMIDE.....	81(Vol 1)
CF4	CARBON TETRAFLUORIDE.....	12(Vol 1)	C2H3Cl	VINYL CHLORIDE.....	82(Vol 1)
CHBr3	TRIBROMOMETHANE.....	13(Vol 1)	C2H3ClF2	1-CHLORO-1,1-DIFLUOROETHANE.....	83(Vol 1)
CHClF2	CHLORODIFLUOROMETHANE.....	14(Vol 1)	C2H3ClO	ACETYL CHLORIDE.....	84(Vol 1)
CHCl2F	DICHLOROFLUOROMETHANE.....	15(Vol 1)	C2H3ClO	CHLOROACETALDEHYDE.....	85(Vol 1)
CHCl3	CHLOROFORM.....	16(Vol 1)	C2H3ClO2	CHLOROACETIC ACID.....	86(Vol 1)
CHF3	TRIFLUOROMETHANE.....	17(Vol 1)	C2H3ClO2	METHYL CHLOROFORMATE.....	87(Vol 1)
CHN	HYDROGEN CYANIDE.....	18(Vol 1)	C2H3Cl3	1,1,1-TRICHLOROETHANE.....	88(Vol 1)
CH2BrCl	BROMOCHLOROMETHANE.....	19(Vol 1)	C2H3Cl3	1,1,2-TRICHLOROETHANE.....	89(Vol 1)
CH2Br2	DIBROMOMETHANE.....	20(Vol 1)	C2H3F	VINYL FLUORIDE.....	90(Vol 1)
CH2Cl2	DICHLOROMETHANE.....	21(Vol 1)	C2H3F3	1,1,1-TRIFLUOROETHANE.....	91(Vol 1)
CH2F2	DIFLUOROMETHANE.....	22(Vol 1)	C2H3N	ACETONITRILE.....	92(Vol 1)
CH2I2	DIIODOMETHANE.....	23(Vol 1)	C2H3NO	METHYL ISOCYANATE.....	93(Vol 1)
CH2O	FORMALDEHYDE.....	24(Vol 1)	C2H4	ETHYLENE.....	94(Vol 1)
CH2O2	FORMIC ACID.....	25(Vol 1)	C2H4Br2	1,1-DIBROMOETHANE.....	95(Vol 1)
CH3Br	METHYL BROMIDE.....	26(Vol 1)	C2H4Br2	1,2-DIBROMOETHANE.....	96(Vol 1)
CH3Cl	METHYL CHLORIDE.....	27(Vol 1)	C2H4Cl2	1,1-DICHLOROETHANE.....	97(Vol 1)
CH3Cl3Si	METHYL TRICHLOROSILANE.....	28(Vol 1)	C2H4Cl2	1,2-DICHLOROETHANE.....	98(Vol 1)
CH3F	METHYL FLUORIDE.....	29(Vol 1)	C2H4Cl2O	BIS(CHLOROMETHYL)ETHER.....	99(Vol 1)
CH3I	METHYL IODIDE.....	30(Vol 1)	C2H4F2	1,1-DIFLUOROETHANE.....	100(Vol 1)
CH3NO	FORMAMIDE.....	31(Vol 1)	C2H4F2	1,2-DIFLUOROETHANE.....	101(Vol 1)
CH3NO2	NITROMETHANE.....	32(Vol 1)	C2H4O	ACETALDEHYDE.....	102(Vol 1)
CH4	METHANE.....	33(Vol 1)	C2H4O	ETHYLENE OXIDE.....	103(Vol 1)
CH4Cl2Si	METHYL DICHLOROSILANE.....	34(Vol 1)	C2H4O2	ACETIC ACID.....	104(Vol 1)
CH4O	METHANOL.....	35(Vol 1)	C2H4O2	METHYL FORMATE.....	105(Vol 1)
CH4O3S	METHANESULFONIC ACID.....	36(Vol 1)	C2H5Br	BROMOETHANE.....	106(Vol 1)
CH4S	METHYL MERCAPTAN.....	37(Vol 1)	C2H5Cl	ETHYL CHLORIDE.....	107(Vol 1)
CH5ClSi	METHYL CHLOROSILANE.....	38(Vol 1)	C2H5ClO	2-CHLOROETHANOL.....	108(Vol 1)
CH5N	METHYLAMINE.....	39(Vol 1)	C2H5F	ETHYL FLUORIDE.....	109(Vol 1)
CH6Si	METHYL SILANE.....	40(Vol 1)	C2H5I	ETHYL IODIDE.....	110(Vol 1)
CN4O8	TETRANITROMETHANE.....	41(Vol 1)	C2H5N	ETHYLENEIMINE.....	111(Vol 1)
CO	CARBON MONOXIDE.....	42(Vol 1)	C2H5NO	ACETAMIDE.....	112(Vol 1)
COS	CARBONYL SULFIDE.....	43(Vol 1)	C2H5NO	N-METHYLFORMAMIDE.....	113(Vol 1)
CO2	CARBON DIOXIDE.....	44(Vol 1)	C2H5NO2	NITROETHANE.....	114(Vol 1)
CS2	CARBON DISULFIDE.....	45(Vol 1)	C2H6	ETHANE.....	115(Vol 1)
C2BrF3	BROMOTRIFLUOROETHYLENE.....	46(Vol 1)	C2H6AlCl	DIMETHYLALUMINUM CHLORIDE.....	116(Vol 1)
C2BrF2F4	1,2-DIBROMOTETRAFLUOROETHANE.....	47(Vol 1)	C2H6O	DIMETHYL ETHER.....	117(Vol 1)
C2ClF3	CHLOROTRIFLUOROETHYLENE.....	48(Vol 1)	C2H6O	ETHANOL.....	118(Vol 1)
C2ClF5	CHLOROPENTAFLUOROETHANE.....	49(Vol 1)	C2H6OS	DIMETHYL SULFOXIDE.....	119(Vol 1)
C2Cl2F4	1,2-DICHLOROTETRAFLUOROETHANE.....	50(Vol 1)	C2H6O2	ETHYLENE GLYCOL.....	120(Vol 1)
C2Cl3F3	1,1,2-TRICHLOROTRIFLUOROETHANE.....	51(Vol 1)	C2H6O4S	DIMETHYL SULFATE.....	121(Vol 1)
C2Cl4	TETRACHLOROETHYLENE.....	52(Vol 1)	C2H6S	DIMETHYL SULFIDE.....	122(Vol 1)
C2Cl4F2	1,1,2,2-TETRACHLORODIFLUOROETHANE.....	53(Vol 1)	C2H6S	ETHYL MERCAPTAN.....	123(Vol 1)
C2Cl4O	TRICHLOROACETYL CHLORIDE.....	54(Vol 1)	C2H6S2	DIMETHYL DISULFIDE.....	124(Vol 1)
C2Cl6	HEXACHLOROETHANE.....	55(Vol 1)	C2H7N	DIMETHYLAMINE.....	125(Vol 1)
C2F4	TETRAFLUOROETHYLENE.....	56(Vol 1)	C2H7N	ETHYLAMINE.....	126(Vol 1)
C2F6	HEXAFLUOROETHANE.....	57(Vol 1)	C2H7NO	MONOETHANOLAMINE.....	127(Vol 1)
C2HBrClF3	HALOTHANE.....	58(Vol 1)	C2H8N2	ETHYLENEDIAMINE.....	128(Vol 1)
C2HClF2	2-CHLORO-1,1-DIFLUOROETHYLENE.....	59(Vol 1)	C2H8Si	DIMETHYL SILANE.....	129(Vol 1)
C2HCl3	TRICHLOROETHYLENE.....	60(Vol 1)	C2N2	CYANOGEN.....	130(Vol 1)
C2HCl3O	DICHLOROACETYL CHLORIDE.....	61(Vol 1)	C3F6	HEXAFLUOROPROPYLENE.....	131(Vol 1)
C2HCl3O	TRICHLOROACETALDEHYDE.....	62(Vol 1)	C3F6O	HEXAFLUOROACETONE.....	132(Vol 1)
C2HCl5	PENTACHLOROETHANE.....	63(Vol 1)	C3F8	OCTAFLUOROPROPANE.....	133(Vol 1)
C2HF3O2	TRIFLUOROACETIC ACID.....	64(Vol 1)	C3H2N2	MALONONITRILE.....	134(Vol 1)
C2HF5	PENTAFLUOROETHANE.....	65(Vol 1)	C3H3Cl	PROPARGYL CHLORIDE.....	135(Vol 1)
C2H2	ACETYLENE.....	66(Vol 1)	C3H3N	ACRYLONITRILE.....	136(Vol 1)
C2H2Br4	1,1,2,2-TETRABROMOETHANE.....	67(Vol 1)	C3H3NO	OXAZOLE.....	137(Vol 1)
C2H2Cl2	1,1-DICHLOROETHYLENE.....	68(Vol 1)	C3H4	METHYLACETYLENE.....	138(Vol 1)
C2H2Cl2	cis-1,2-DICHLOROETHYLENE.....	69(Vol 1)	C3H4	PROPADIENE.....	139(Vol 1)
C2H2Cl2	trans-1,2-DICHLOROETHYLENE.....	70(Vol 1)	C3H4Cl2	2,3-DICHLOROPROPENE.....	140(Vol 1)

C3H4O	ACROLEIN.....	141(Vol 1)	C4H4O3	SUCCINIC ANHYDRIDE.....	219(Vol 1)
C3H4O	PROPARGYL ALCOHOL.....	142(Vol 1)	C4H4O4	FUMARIC ACID.....	220(Vol 1)
C3H4O2	ACRYLIC ACID.....	143(Vol 1)	C4H4O4	MALEIC ACID.....	221(Vol 1)
C3H4O2	BETA-PROPIOLACTONE.....	144(Vol 1)	C4H4S	THIOPHENE.....	222(Vol 1)
C3H4O2	VINYL FORMATE.....	145(Vol 1)	C4H5Cl	CHLOROPRENE.....	223(Vol 1)
C3H4O3	ETHYLENE CARBONATE.....	146(Vol 1)	C4H5N	trans-CROTONITRILE.....	224(Vol 1)
C3H4O3	PYRUVIC ACID.....	147(Vol 1)	C4H5N	cis-CROTONITRILE.....	225(Vol 1)
C3H5Cl	2-CHLOROPROPENE.....	148(Vol 1)	C4H5N	METHACRYLONITRILE.....	226(Vol 1)
C3H5Cl	3-CHLOROPROPENE.....	149(Vol 1)	C4H5N	PYRROLE.....	227(Vol 1)
C3H5ClO	alpha-EPICHLOROHYDRIN.....	150(Vol 1)	C4H5N	VINYLACTIONITRILE.....	228(Vol 1)
C3H5ClO2	METHYL CHLOROACETATE.....	151(Vol 1)	C4H5NO2	METHYL CYANOACETATE.....	229(Vol 1)
C3H5ClO2	ETHYL CHLOROFORMATE.....	152(Vol 1)	C4H6	1,2-BUTADIENE.....	230(Vol 1)
C3H5Cl3	1,2,3-TRICHLOROPROPANE.....	153(Vol 1)	C4H6	1,3-BUTADIENE.....	231(Vol 1)
C3H5N	PROPIONITRILE.....	154(Vol 1)	C4H6	DIMETHYLACETYLENE.....	232(Vol 1)
C3H5NO	ACRYLAMIDE.....	155(Vol 1)	C4H6	ETHYLACETYLENE.....	233(Vol 1)
C3H5NO	HYDRACRYLONITRILE.....	156(Vol 1)	C4H6Cl2	1,3-DICHLORO-trans-2-BUTENE.....	234(Vol 1)
C3H5NO	LACTONITRILE.....	157(Vol 1)	C4H6Cl2	1,4-DICHLORO-cis-2-BUTENE.....	235(Vol 1)
C3H5N3O9	NITROGLYCERINE.....	158(Vol 1)	C4H6Cl2	1,4-DICHLORO-trans-2-BUTENE.....	236(Vol 1)
C3H6	CYCLOPROPANE.....	159(Vol 1)	C4H6Cl2	3,4-DICHLORO-1-BUTENE.....	237(Vol 1)
C3H6	PROPYLENE.....	160(Vol 1)	C4H6O	trans-CROTONALDEHYDE.....	238(Vol 1)
C3H6Cl2	1,1-DICHLOROPROPANE.....	161(Vol 1)	C4H6O	2,5-DIHYDROFURAN.....	239(Vol 1)
C3H6Cl2	1,2-DICHLOROPROPANE.....	162(Vol 1)	C4H6O	DIVINYL ETHER.....	240(Vol 1)
C3H6Cl2	1,3-DICHLOROPROPANE.....	163(Vol 2)	C4H6O	METHACROLEIN.....	241(Vol 1)
C3H6O	ACETONE.....	164(Vol 1)	C4H6O2	2-BUTYNE-1,4-DIOL.....	242(Vol 1)
C3H6O	ALLYL ALCOHOL.....	165(Vol 1)	C4H6O2	GAMMA-BUTYROLACTONE.....	243(Vol 1)
C3H6O	METHYL VINYL ETHER.....	166(Vol 1)	C4H6O2	cis-CROTONIC ACID.....	244(Vol 1)
C3H6O	n-PROPIONALDEHYDE.....	167(Vol 1)	C4H6O2	trans-CROTONIC ACID.....	245(Vol 1)
C3H6O	1,2-PROPYLENE OXIDE.....	168(Vol 1)	C4H6O2	METHACRYLIC ACID.....	246(Vol 1)
C3H6O	1,3-PROPYLENE OXIDE.....	169(Vol 1)	C4H6O2	METHYL ACRYLATE.....	247(Vol 1)
C3H6O2	ETHYL FORMATE.....	170(Vol 1)	C4H6O2	VINYL ACETATE.....	248(Vol 1)
C3H6O2	METHYL ACETATE.....	171(Vol 1)	C4H6O3	ACETIC ANHYDRIDE.....	249(Vol 1)
C3H6O2	PROPIONIC ACID.....	172(Vol 1)	C4H6O4	SUCCINIC ACID.....	250(Vol 1)
C3H6O2S	3-MERCAPTOPROPIONIC ACID.....	173(Vol 1)	C4H6O5	DIGLYCOLIC ACID.....	251(Vol 1)
C3H6O3	LACTIC ACID.....	174(Vol 1)	C4H6O5	MALIC ACID.....	252(Vol 1)
C3H6O3	METHOXYACETIC ACID.....	175(Vol 1)	C4H6O6	TARTARIC ACID.....	253(Vol 1)
C3H6O3	TRIOXANE.....	176(Vol 1)	C4H7N	n-BUTYRONITRILE.....	254(Vol 1)
C3H7Br	1-BROMOPROPANE.....	177(Vol 1)	C4H7N	ISOBUTYRONITRILE.....	255(Vol 1)
C3H7Br	2-BROMOPROPANE.....	178(Vol 1)	C4H7NO	ACETONE CYANOHYDRIN.....	256(Vol 1)
C3H7Cl	ISOPROPYL CHLORIDE.....	179(Vol 1)	C4H7NO	2-METHACRYLAMIDE.....	257(Vol 1)
C3H7Cl	n-PROPYL CHLORIDE.....	180(Vol 1)	C4H7NO	3-METHOXYPROPIONITRILE.....	258(Vol 1)
C3H7I	ISOPROPYL IODIDE.....	181(Vol 1)	C4H7NO	2-PYRROLIDONE.....	259(Vol 1)
C3H7I	n-PROPYL IODIDE.....	182(Vol 1)	C4H8	1-BUTENE.....	260(Vol 1)
C3H7N	ALLYLAMINE.....	183(Vol 1)	C4H8	cis-2-BUTENE.....	261(Vol 1)
C3H7N	PROPYLENEIMINE.....	184(Vol 1)	C4H8	trans-2-BUTENE.....	262(Vol 1)
C3H7NO	N,N-DIMETHYLFORMAMIDE.....	185(Vol 1)	C4H8	CYCLOBUTANE.....	263(Vol 1)
C3H7NO	N-METHYLACETAMIDE.....	186(Vol 1)	C4H8	ISOBUTENE.....	264(Vol 1)
C3H7NO2	1-NITROPROPANE.....	187(Vol 1)	C4H8Cl2	1,4-DICHLOROBUTANE.....	265(Vol 1)
C3H7NO2	2-NITROPROPANE.....	188(Vol 1)	C4H8O	n-BUTYRALDEHYDE.....	266(Vol 1)
C3H8	PROPANE.....	189(Vol 1)	C4H8O	ISOBUTYRALDEHYDE.....	267(Vol 1)
C3H8O	ISOPROPANOL.....	190(Vol 1)	C4H8O	1,2-EPOXYBUTANE.....	268(Vol 1)
C3H8O	METHYL ETHYL ETHER.....	191(Vol 1)	C4H8O	METHYL ETHYL KETONE.....	269(Vol 1)
C3H8O	n-PROPANOL.....	192(Vol 1)	C4H8O	ETHYL VINYL ETHER.....	270(Vol 1)
C3H8O2	2-METHOXYETHANOL.....	193(Vol 1)	C4H8O	TETRAHYDROFURAN.....	271(Vol 1)
C3H8O2	METHYLAL.....	194(Vol 1)	C4H8O2	cis-2-BUTENE-1,4-DIOL.....	272(Vol 1)
C3H8O2	1,2-PROPYLENE GLYCOL.....	195(Vol 1)	C4H8O2	trans-2-BUTENE-1,4-DIOL.....	273(Vol 1)
C3H8O2	1,3-PROPYLENE GLYCOL.....	196(Vol 1)	C4H8O2	ISOBUTYRIC ACID.....	274(Vol 1)
C3H8O3	GLYCEROL.....	197(Vol 1)	C4H8O2	n-BUTYRIC ACID.....	275(Vol 1)
C3H8S	n-PROPYLMERCAPTAN.....	198(Vol 1)	C4H8O2	1,4-DIOXANE.....	276(Vol 1)
C3H8S	ISOPROPYL MERCAPTAN.....	199(Vol 1)	C4H8O2	ETHYL ACETATE.....	277(Vol 1)
C3H9N	n-PROPYLAMINE.....	200(Vol 1)	C4H8O2	METHYL PROPIONATE.....	278(Vol 1)
C3H9N	ISOPROPYLAMINE.....	201(Vol 1)	C4H8O2	n-PROPYL FORMATE.....	279(Vol 1)
C3H9N	TRIMETHYLAMINE.....	202(Vol 1)	C4H8O2S	SULFOLANE.....	280(Vol 1)
C3H9NO	1-AMINO-2-PROPANOL.....	203(Vol 1)	C4H8S	TETRAHYDROTHIOPHENE.....	281(Vol 1)
C3H9NO	3-AMINO-1-PROPANOL.....	204(Vol 1)	C4H9Br	1-BROMOBUTANE.....	282(Vol 1)
C3H9NO	METHYLETHANOLAMINE.....	205(Vol 1)	C4H9Br	2-BROMOBUTANE.....	283(Vol 1)
C3H9O4P	TRIMETHYL PHOSPHATE.....	206(Vol 1)	C4H9Cl	n-BUTYL CHLORIDE.....	284(Vol 1)
C3H10N2	1,2-PROPANEDIAMINE.....	207(Vol 1)	C4H9Cl	sec-BUTYL CHLORIDE.....	285(Vol 1)
C3H10Si	TRIMETHYL SILANE.....	208(Vol 1)	C4H9Cl	tert-BUTYL CHLORIDE.....	286(Vol 1)
C4Cl4S	TETRACHLOROTHIOPHENE.....	209(Vol 1)	C4H9N	PYRROLIDINE.....	287(Vol 1)
C4Cl6	HEXACHLORO-1,3-BUTADIENE.....	210(Vol 1)	C4H9NO	N,N-DIMETHYLACETAMIDE.....	288(Vol 1)
C4F8	OCTAFLUORO-2-BUTENE.....	211(Vol 1)	C4H9NO	MORPHOLINE.....	289(Vol 1)
C4F8	OCTAFLUOROCYCLOBUTANE.....	212(Vol 1)	C4H10	n-BUTANE.....	290(Vol 1)
C4F10	DECAFLUOROBUTANE.....	213(Vol 1)	C4H10	ISOBUTANE.....	291(Vol 1)
C4H2O3	MALEIC ANHYDRIDE.....	214(Vol 1)	C4H10N2	PIPERAZINE.....	292(Vol 1)
C4H4	VINYLAETYLENE.....	215(Vol 1)	C4H10O	n-BUTANOL.....	293(Vol 1)
C4H4N2	SUCCINONITRILE.....	216(Vol 1)	C4H10O	sec-BUTANOL.....	294(Vol 1)
C4H4O	FURAN.....	217(Vol 1)	C4H10O	tert-BUTANOL.....	295(Vol 1)
C4H4O2	DIKETENE.....	218(Vol 1)	C4H10O	DIETHYL ETHER.....	296(Vol 1)

C4H100	METHYL ISOPROPYL ETHER.....	297(Vol 1)	C5H100	VALERALDEHYDE.....	52(Vol 2)
C4H100	ISOBUTANOL.....	298(Vol 1)	C5H1002	n-BUTYL FORMATE.....	53(Vol 2)
C4H1002	1,3-BUTANEDIOL.....	299(Vol 1)	C5H1002	ETHYL PROPIONATE.....	54(Vol 2)
C4H1002	1,4-BUTANEDIOL.....	300(Vol 1)	C5H1002	ISOBUTYL FORMATE.....	55(Vol 2)
C4H1002	2,3-BUTANEDIOL.....	301(Vol 1)	C5H1002	ISOPROPYL ACETATE.....	56(Vol 2)
C4H1002	t-BUTYL HYDROPEROXIDE.....	302(Vol 1)	C5H1002	n-PROPYL ACETATE.....	57(Vol 2)
C4H1002	1,2-DIMETHOXYETHANE.....	303(Vol 1)	C5H1002	METHYL n-BUTYRATE.....	58(Vol 2)
C4H1002	2-ETHOXYETHANOL.....	304(Vol 1)	C5H1002	2-METHYLBUTYRIC ACID.....	59(Vol 2)
C4H1003	DIETHYLENE GLYCOL.....	305(Vol 1)	C5H1002	ISOVALERIC ACID.....	60(Vol 2)
C4H1004S	DIETHYL SULFATE.....	306(Vol 1)	C5H1002	VALERIC ACID.....	61(Vol 2)
C4H10S	n-BUTYL MERCAPTAN.....	307(Vol 1)	C5H1002	TETRAHYDROFURFURYL ALCOHOL.....	62(Vol 2)
C4H10S	ISOBUTYL MERCAPTAN.....	308(Vol 1)	C5H1002S	3-METHYL SULFOLANE.....	63(Vol 2)
C4H10S	sec-BUTYL MERCAPTAN.....	309(Vol 1)	C5H1003	DIETHYL CARBONATE.....	64(Vol 2)
C4H10S	tert-BUTYL MERCAPTAN.....	310(Vol 1)	C5H1003	ETHYL LACTATE.....	65(Vol 2)
C4H10S	DIETHYL SULFIDE.....	311(Vol 1)	C5H11Cl	1-CHLOROPENTANE.....	66(Vol 2)
C4H10S2	DIETHYL DISULFIDE.....	312(Vol 1)	C5H11N	N-METHYLPYRROLIDINE.....	67(Vol 2)
C4H11N	n-BUTYLAMINE.....	313(Vol 1)	C5H11N	PIPERIDINE.....	68(Vol 2)
C4H11N	ISOBUTYLAMINE.....	314(Vol 1)	C5H11NO	tert-BUTYLFORMAMIDE.....	69(Vol 2)
C4H11N	sec-BUTYLAMINE.....	315(Vol 1)	C5H12	ISOPENTANE.....	70(Vol 2)
C4H11N	tert-BUTYLAMINE.....	316(Vol 1)	C5H12	NEOPENTANE.....	71(Vol 2)
C4H11N	DIETHYLAMINE.....	317(Vol 1)	C5H12	n-PENTANE.....	72(Vol 2)
C4H11NO	DIMETHYLETHANOLAMINE.....	318(Vol 1)	C5H120	2,2-DIMETHYL-1-PROPANOL.....	73(Vol 2)
C4H11NO2	DIETHANOLAMINE.....	319(Vol 1)	C5H120	2-METHYL-1-BUTANOL.....	74(Vol 2)
C4H11NO4	2-AMINOETHOXYETHANOL.....	320(Vol 1)	C5H120	2-METHYL-2-BUTANOL.....	75(Vol 2)
C4H12N2O	N-AMINOETHYL ETHANOLAMINE.....	321(Vol 1)	C5H120	3-METHYL-1-BUTANOL.....	76(Vol 2)
C4H12Si	TETRAMETHYLSILANE.....	322(Vol 1)	C5H120	3-METHYL-2-BUTANOL.....	77(Vol 2)
C4H13N3	DIETHYLENE TRIAMINE.....	323(Vol 1)	C5H120	1-PENTANOL.....	78(Vol 2)
C5Cl6	HEXACHLOROXYCYCLOPENTADIENE.....	1(Vol 2)	C5H120	2-PENTANOL.....	79(Vol 2)
C5H4O2	FURFURAL.....	2(Vol 2)	C5H120	3-PENTANOL.....	80(Vol 2)
C5H5N	PYRIDINE.....	3(Vol 2)	C5H120	METHYL sec-BUTYL ETHER.....	81(Vol 2)
C5H6	CYCLOPENTADIENE.....	4(Vol 2)	C5H120	METHYL tert-BUTYL ETHER.....	82(Vol 2)
C5H6	2-METHYL-1-BUTENE-3-YNE.....	5(Vol 2)	C5H120	METHYL ISOBUTYL ETHER.....	83(Vol 2)
C5H6	1-PENTENE-3-YNE.....	6(Vol 2)	C5H120	ETHYL PROPYL ETHER.....	84(Vol 2)
C5H6	1-PENTENE-4-YNE.....	7(Vol 2)	C5H1202	ETHYLENE GLYCOL MONOPROPYL ETHER.....	85(Vol 2)
C5H6N2	GLUTARONITRILE.....	8(Vol 2)	C5H1202	NEOPENTYL GLYCOL.....	86(Vol 2)
C5H6O2	FURFURYL ALCOHOL.....	9(Vol 2)	C5H1202	1,5-PENTANEDIOL.....	87(Vol 2)
C5H6O3	GLUTARIC ANHYDRIDE.....	10(Vol 2)	C5H1203	2-(2-METHOXYETHOXY)ETHANOL.....	88(Vol 2)
C5H6O4	CITRACONIC ACID.....	11(Vol 2)	C5H1204	PENTAERYTHRITOL.....	89(Vol 2)
C5H7N	N-METHYLPYRROLE.....	13(Vol 2)	C5H12S	n-PENTYL MERCAPTAN.....	90(Vol 2)
C5H7NO2	ETHYL CYANOACETATE.....	14(Vol 2)	C5H13N	n-PENTYLAMINE.....	91(Vol 2)
C5H8	CYCLOPENTENE.....	15(Vol 2)	C5H13NO2	METHYL DIETHANOLAMINE.....	92(Vol 2)
C5H8	ISOPRENE.....	16(Vol 2)	C6Cl6	HEXACHLORO BENZENE.....	93(Vol 2)
C5H8	3-METHYL-1,2-BUTADIENE.....	17(Vol 2)	C6F6	HEXAFLUOROBENZENE.....	94(Vol 2)
C5H8	1,2-PENTADIENE.....	18(Vol 2)	C6H3ClN2O4	1-CHLORO-2,4-DINITROBENZENE.....	95(Vol 2)
C5H8	cis-1,3-PENTADIENE.....	19(Vol 2)	C6H3Cl2NO2	1,2-DICHLORO-4-NITROBENZENE.....	96(Vol 2)
C5H8	trans-1,3-PENTADIENE.....	20(Vol 2)	C6H3Cl3	1,2,4-TRICHLOROBENZENE.....	97(Vol 2)
C5H8	1,4-PENTADIENE.....	21(Vol 2)	C6H3N3O6	1,3,5-TRINITROBENZENE.....	98(Vol 2)
C5H8	2,3-PENTADIENE.....	22(Vol 2)	C6H4Br2	m-DIBROMOBENZENE.....	99(Vol 2)
C5H8	1-PENTYNE.....	23(Vol 2)	C6H4ClNO2	m-CHLORONITROBENZENE.....	100(Vol 2)
C5H8	3-METHYL-1-BUTYNE.....	24(Vol 2)	C6H4ClNO2	o-CHLORONITROBENZENE.....	101(Vol 2)
C5H8N4O12	PENTAERYTHRITOL TETRANITRATE.....	25(Vol 2)	C6H4ClNO2	p-CHLORONITROBENZENE.....	102(Vol 2)
C5H8O	CYCLOPENTANONE.....	26(Vol 2)	C6H4Cl2	m-DICHLOROBENZENE.....	103(Vol 2)
C5H8O	METHYL ISOPROPENYL KETONE.....	27(Vol 2)	C6H4Cl2	o-DICHLOROBENZENE.....	104(Vol 2)
C5H8O2	ACETYLACETONE.....	28(Vol 2)	C6H4Cl2	p-DICHLOROBENZENE.....	105(Vol 2)
C5H8O2	ALLYL ACETATE.....	29(Vol 2)	C6H4N2O4	m-DINITROBENZENE.....	106(Vol 2)
C5H8O2	ETHYL ACRYLATE.....	30(Vol 2)	C6H4N2O4	o-DINITROBENZENE.....	107(Vol 2)
C5H8O2	METHYL METHACRYLATE.....	31(Vol 2)	C6H4N2O4	p-DINITROBENZENE.....	108(Vol 2)
C5H8O2	VINYL PROPIONATE.....	32(Vol 2)	C6H5Br	BROMOBENZENE.....	109(Vol 2)
C5H8O3	2-HYDROXYETHYL ACRYLATE.....	33(Vol 2)	C6H5Cl	MONOCHLOROBENZENE.....	110(Vol 2)
C5H8O3	LEVULINIC ACID.....	34(Vol 2)	C6H5ClO	m-CHLOROPHENOL.....	111(Vol 2)
C5H8O3	METHYL ACETOACETATE.....	35(Vol 2)	C6H5ClO	o-CHLOROPHENOL.....	112(Vol 2)
C5H8O4	GLUTARIC ACID.....	36(Vol 2)	C6H5ClO	p-CHLOROPHENOL.....	113(Vol 2)
C5H9N	VALERONITRILE.....	37(Vol 2)	C6H5Cl2N	3,4-DICHLOROANILINE.....	114(Vol 2)
C5H9NO	n-BUTYL ISOCYANATE.....	38(Vol 2)	C6H5F	FLUOROBENZENE.....	115(Vol 2)
C5H9NO	N-METHYL-2-PYRROLIDONE.....	39(Vol 2)	C6H5I	IODOBENZENE.....	116(Vol 2)
C5H9NO4	L-GLUTAMIC ACID.....	40(Vol 2)	C6H5NO2	NITROBENZENE.....	117(Vol 2)
C5H10	CYCLOPENTANE.....	41(Vol 2)	C6H6	BENZENE.....	118(Vol 2)
C5H10	2-METHYL-1-BUTENE.....	42(Vol 2)	C6H6ClN	m-CHLOROANILINE.....	119(Vol 2)
C5H10	2-METHYL-2-BUTENE.....	43(Vol 2)	C6H6ClN	o-CHLOROANILINE.....	120(Vol 2)
C5H10	3-METHYL-1-BUTENE.....	44(Vol 2)	C6H6ClN	p-CHLOROANILINE.....	121(Vol 2)
C5H10	1-PENTENE.....	45(Vol 2)	C6H6N2	cis-DICYANO-1-BUTENE.....	122(Vol 2)
C5H10	cis-2-PENTENE.....	46(Vol 2)	C6H6N2	trans-DICYANO-1-BUTENE.....	123(Vol 2)
C5H10	trans-2-PENTENE.....	47(Vol 2)	C6H6N2	1,4-DICYANO-2-BUTENE.....	124(Vol 2)
C5H10Cl2	1,5-DICHLOROPENTANE.....	48(Vol 2)	C6H6N2O2	m-NITROANILINE.....	125(Vol 2)
C5H100	METHYL ISOPROPYL KETONE.....	49(Vol 2)	C6H6N2O2	o-NITROANILINE.....	126(Vol 2)
C5H100	2-PENTANONE.....	50(Vol 2)	C6H6N2O2	p-NITROANILINE.....	127(Vol 2)
C5H100	DIETHYL KETONE.....	51(Vol 2)	C6H6O	PHENOL.....	128(Vol 2)
			C6H6O2	1,2-BENZENEDIOL.....	129(Vol 2)

C6H6O2	1,3-BENZENEDIOL.....	130(Vol 2)	C6H12O2	2-ETHYL BUTYRIC ACID.....	208(Vol 2)
C6H6O2	p-HYDROQUINONE.....	131(Vol 2)	C6H12O2	n-HEXANOIC ACID.....	209(Vol 2)
C6H6O3	1,2,3-BENZENETRIOL.....	132(Vol 2)	C6H12O3	2-ETHOXYETHYL ACETATE.....	210(Vol 2)
C6H6S	PHENYL MERCAPTAN.....	133(Vol 2)	C6H12O3	HYDROXYCAPROIC ACID.....	211(Vol 2)
C6H7N	ANILINE.....	134(Vol 2)	C6H12O3	PARALDEHYDE.....	212(Vol 2)
C6H7N	2-METHYLPYRIDINE.....	135(Vol 2)	C6H12O3	sec-BUTYL GLYCOLATE.....	213(Vol 2)
C6H7N	3-METHYLPYRIDINE.....	136(Vol 2)	C6H13N	CYCLOHEXYLAMINE.....	214(Vol 2)
C6H7N	4-METHYLPYRIDINE.....	137(Vol 2)	C6H13N	HEXAMETHYLENEIMINE.....	215(Vol 2)
C6H8	1,3-CYCLOHEXADIENE.....	138(Vol 2)	C6H14	2,2-DIMETHYLBUTANE.....	216(Vol 2)
C6H8	METHYLCYCLOPENTADIENE.....	139(Vol 2)	C6H14	2,3-DIMETHYLBUTANE.....	217(Vol 2)
C6H8N2	ADIPONITRILE.....	140(Vol 2)	C6H14	n-HEXANE.....	218(Vol 2)
C6H8N2	METHYLGUTARONITRILE.....	141(Vol 2)	C6H14	2-METHYLPENTANE.....	219(Vol 2)
C6H8N2	m-PHENYLENEDIAMINE.....	142(Vol 2)	C6H14	3-METHYLPENTANE.....	220(Vol 2)
C6H8N2	o-PHENYLENEDIAMINE.....	143(Vol 2)	C6H14N2O2	LYSINE.....	221(Vol 2)
C6H8N2	p-PHENYLENEDIAMINE.....	144(Vol 2)	C6H14O	2-ETHYL-1-BUTANOL.....	222(Vol 2)
C6H8N2	PHENYLHYDRAZINE.....	145(Vol 2)	C6H14O	1-HEXANOL.....	223(Vol 2)
C6H8N2O	BIS(CYANOETHYL)ETHER.....	146(Vol 2)	C6H14O	2-HEXANOL.....	224(Vol 2)
C6H8O4	DIMETHYL MALEATE.....	147(Vol 2)	C6H14O	2-METHYL-1-PENTANOL.....	225(Vol 2)
C6H8O6	ASCORBIC ACID.....	148(Vol 2)	C6H14O	4-METHYL-2-PENTANOL.....	226(Vol 2)
C6H8O7	CITRIC ACID.....	149(Vol 2)	C6H14O	n-BUTYL ETHYL ETHER.....	227(Vol 2)
C6H10	CYCLOHEXENE.....	150(Vol 2)	C6H14O	DIISOPROPYL ETHER.....	228(Vol 2)
C6H10	2,3-DIMETHYL-1,3-BUTADIENE.....	151(Vol 2)	C6H14O	DI-n-PROPYL ETHER.....	229(Vol 2)
C6H10	1,5-HEXADIENE.....	152(Vol 2)	C6H14O	METHYL tert-PENTYL ETHER.....	230(Vol 2)
C6H10	cis,trans-2,4-HEXADIENE.....	153(Vol 2)	C6H14O2	ACETAL.....	231(Vol 2)
C6H10	trans,trans-2,4-HEXADIENE.....	154(Vol 2)	C6H14O2	2-BUTOXYETHANOL.....	232(Vol 2)
C6H10	1-HEXYNE.....	155(Vol 2)	C6H14O2	1,6-HEXANEDIOL.....	233(Vol 2)
C6H10	2-HEXYNE.....	156(Vol 2)	C6H14O2	HEXYLENE GLYCOL.....	234(Vol 2)
C6H10	3-HEXYNE.....	157(Vol 2)	C6H14O2S	DI-n-PROPYL SULFONE.....	235(Vol 2)
C6H10O	CYCLOHEXANONE.....	158(Vol 2)	C6H14O3	DIETHYLENE GLYCOL DIMETHYL ETHER.....	236(Vol 2)
C6H10O	MESITYL OXIDE.....	159(Vol 2)	C6H14O3	DIPROPYLENE GLYCOL.....	237(Vol 2)
C6H10O2	epsilon-CAPROLACTONE.....	160(Vol 2)	C6H14O3	2-(2-ETHOXYETHOXY)ETHANOL.....	238(Vol 2)
C6H10O2	ETHYL METHACRYLATE.....	161(Vol 2)	C6H14O3	TRIMETHYLOLPROPANE.....	239(Vol 2)
C6H10O3	n-PROPYL ACRYLATE.....	162(Vol 2)	C6H14O4	TRIETHYLENE GLYCOL.....	240(Vol 2)
C6H10O3	ETHYLACETOACETATE.....	163(Vol 2)	C6H14O6	SORBITOL.....	241(Vol 2)
C6H10O3	PROPIONIC ANHYDRIDE.....	164(Vol 2)	C6H14S	n-HEXYLMERCAPTAN.....	242(Vol 2)
C6H10O4	ADIPIC ACID.....	165(Vol 2)	C6H15Al	TRIETHYL ALUMINUM.....	243(Vol 2)
C6H10O4	DIETHYL OXALATE.....	166(Vol 2)	C6H15Al2Cl3	ETHYL ALUMINUM SESQUICHLORIDE.....	244(Vol 2)
C6H10O4	ETHYLENE GLYCOL DIACETATE.....	167(Vol 2)	C6H15N	DIISOPROPYLAMINE.....	245(Vol 2)
C6H10O4	ETHYLIDENE DIACETATE.....	168(Vol 2)	C6H15N	DI-n-PROPYLAMINE.....	246(Vol 2)
C6H11N	HEXANENITRILE.....	169(Vol 2)	C6H15N	n-HEXYLAMINE.....	247(Vol 2)
C6H11NO	epsilon-CAPROLACTAM.....	170(Vol 2)	C6H15N	TRIETHYLAMINE.....	248(Vol 2)
C6H11NO	CYCLOHEXANONE OXIME.....	171(Vol 2)	C6H15NO	6-AMINOHEXANOL.....	249(Vol 2)
C6H12	CYCLOHEXANE.....	172(Vol 2)	C6H15NO2	DIISOPROPANOLAMINE.....	250(Vol 2)
C6H12	2,3-DIMETHYL-1-BUTENE.....	173(Vol 2)	C6H15NO3	TRIETHANOLAMINE.....	251(Vol 2)
C6H12	2,3-DIMETHYL-2-BUTENE.....	174(Vol 2)	C6H15N3	N-AMINOETHYL PIPERAZINE.....	252(Vol 2)
C6H12	3,3-DIMETHYL-1-BUTENE.....	175(Vol 2)	C6H15O4P	TRIETHYL PHOSPHATE.....	253(Vol 2)
C6H12	2-ETHYL-1-BUTENE.....	176(Vol 2)	C6H16N2	HEXAMETHYLENEDIAMINE.....	254(Vol 2)
C6H12	1-HEXENE.....	177(Vol 2)	C6H18N3OP	HEXAMETHYL PHOSPHORAMIDE.....	255(Vol 2)
C6H12	cis-2-HEXENE.....	178(Vol 2)	C6H18N4	TRIETHYLENE TETRAMINE.....	256(Vol 2)
C6H12	trans-2-HEXENE.....	179(Vol 2)	C6H18OSi2	HEXAMETHYLDISILOXANE.....	257(Vol 2)
C6H12	cis-3-HEXENE.....	180(Vol 2)	C6H18O3Si3	HEXAMETHYLCYCLOTETRISILOXANE.....	258(Vol 2)
C6H12	trans-3-HEXENE.....	181(Vol 2)	C6H19NSi2	HEXAMETHYLDISILOXANE.....	259(Vol 2)
C6H12	METHYLCYCLOPENTANE.....	182(Vol 2)	C7H3ClF3NO2	4-CHLORO-3-NITROBENZOTRIFLUORIDE.....	260(Vol 2)
C6H12	2-METHYL-1-PENTENE.....	183(Vol 2)	C7H3Cl2F3	2,4-DICHLOROBENZOTRIFLUORIDE.....	261(Vol 2)
C6H12	2-METHYL-2-PENTENE.....	184(Vol 2)	C7H3Cl2NO	3,4-DICHLOROPHENYL ISOCYANATE.....	262(Vol 2)
C6H12	3-METHYL-1-PENTENE.....	185(Vol 2)	C7H4ClF3	p-CHLOROBENZOTRIFLUORIDE.....	263(Vol 2)
C6H12	3-METHYL-cis-2-PENTENE.....	186(Vol 2)	C7H4Cl2O	m-CHLOROBENZOYL CHLORIDE.....	264(Vol 2)
C6H12	4-METHYL-1-PENTENE.....	187(Vol 2)	C7H4F3NO2	3-NITROBENZOTRIFLUORIDE.....	265(Vol 2)
C6H12	4-METHYL-cis-2-PENTENE.....	188(Vol 2)	C7H5ClO	BENZOYL CHLORIDE.....	266(Vol 2)
C6H12	4-METHYL-trans-2-PENTENE.....	189(Vol 2)	C7H5ClO2	o-CHLOROBENZOIC ACID.....	267(Vol 2)
C6H12N2	TRIETHYLENEDIAMINE.....	190(Vol 2)	C7H5Cl3	BENZOTRICHLORIDE.....	268(Vol 2)
C6H12O	BUTYL VINYL ETHER.....	191(Vol 2)	C7H5F3	BENZOTRIFLUORIDE.....	269(Vol 2)
C6H12O	CYCLOHEXANOL.....	192(Vol 2)	C7H5N	BENZONITRILE.....	270(Vol 2)
C6H12O	1-HEXANAL.....	193(Vol 2)	C7H5NO	PHENYL ISOCYANATE.....	271(Vol 2)
C6H12O	ETHYL ISOPROPYL KETONE.....	194(Vol 2)	C7H5N3O6	2,4,6-TRINITROTOLUENE.....	272(Vol 2)
C6H12O	2-HEXANONE.....	195(Vol 2)	C7H6Cl2	BENZYL DICHLORIDE.....	273(Vol 2)
C6H12O	3-HEXANONE.....	196(Vol 2)	C7H6Cl2	2,4-DICHLOROTOLUENE.....	274(Vol 2)
C6H12O	METHYL ISOBUTYL KETONE.....	197(Vol 2)	C7H6N2O4	2,4-DINITROTOLUENE.....	275(Vol 2)
C6H12O2	n-PENTYL FORMATE.....	198(Vol 2)	C7H6N2O4	2,5-DINITROTOLUENE.....	276(Vol 2)
C6H12O2	n-BUTYL ACETATE.....	199(Vol 2)	C7H6N2O4	2,6-DINITROTOLUENE.....	277(Vol 2)
C6H12O2	sec-BUTYL ACETATE.....	200(Vol 2)	C7H6N2O4	3,4-DINITROTOLUENE.....	278(Vol 2)
C6H12O2	tert-BUTYL ACETATE.....	201(Vol 2)	C7H6N2O4	3,5-DINITROTOLUENE.....	279(Vol 2)
C6H12O2	ETHYL n-BUTYRATE.....	202(Vol 2)	C7H6O	BENZALDEHYDE.....	280(Vol 2)
C6H12O2	ETHYL ISOBUTYRATE.....	203(Vol 2)	C7H6O2	BENZOIC ACID.....	281(Vol 2)
C6H12O2	ISOBUTYL ACETATE.....	204(Vol 2)	C7H6O2	p-HYDROXYBENZALDEHYDE.....	282(Vol 2)
C6H12O2	n-PROPYL PROPIONATE.....	205(Vol 2)	C7H6O2	SALICYLALDEHYDE.....	283(Vol 2)
C6H12O2	CYCLOHEXYL PEROXIDE.....	206(Vol 2)	C7H6O3	SALICYLIC ACID.....	284(Vol 2)
C6H12O2	DIACETONE ALCOHOL.....	207(Vol 2)	C7H7Br	p-BROMOTOLUENE.....	285(Vol 2)

C7H7Cl	BENZYL CHLORIDE.....	286(Vol 2)	C7H16O	2-HEPTANOL.....	364(Vol 2)
C7H7Cl	o-CHLOROTOLUENE.....	287(Vol 2)	C7H16O	5-METHYL-1-HEXANOL.....	365(Vol 2)
C7H7Cl	p-CHLOROTOLUENE.....	288(Vol 2)	C7H16S	n-HEPTYL MERCAPTAN.....	366(Vol 2)
C7H7NO	FORMANILIDE.....	289(Vol 2)	C7H17N	1-AMINOHEPTANE.....	367(Vol 2)
C7H7NO2	m-NITROTOLUENE.....	290(Vol 2)	C8H4Cl2O2	ISOPHTHALOYL CHLORIDE.....	1(Vol 3)
C7H7NO2	o-NITROTOLUENE.....	291(Vol 2)	C8H4O3	PHTHALIC ANHYDRIDE.....	2(Vol 3)
C7H7NO2	p-NITROTOLUENE.....	292(Vol 2)	C8H6O4	ISOPHTHALIC ACID.....	3(Vol 3)
C7H7NO3	o-NITROANISOLE.....	293(Vol 2)	C8H6O4	PHTHALIC ACID.....	4(Vol 3)
C7H8	TOLUENE.....	294(Vol 2)	C8H6O4	TEREPHTHALIC ACID.....	5(Vol 3)
C7H8O	ANISOLE.....	295(Vol 2)	C8H6S	BENZOTHIOPHENE.....	6(Vol 3)
C7H8O	BENZYL ALCOHOL.....	296(Vol 2)	C8H7N	INDOLE.....	7(Vol 3)
C7H8O	m-CRESOL.....	297(Vol 2)	C8H8	STYRENE.....	8(Vol 3)
C7H8O	o-CRESOL.....	298(Vol 2)	C8H8O	ACETOPHENONE.....	9(Vol 3)
C7H8O	p-CRESOL.....	299(Vol 2)	C8H8O	p-TOLUALDEHYDE.....	10(Vol 3)
C7H8O2	GUAIACOL.....	300(Vol 2)	C8H8O2	METHYL BENZOATE.....	11(Vol 3)
C7H8O2	p-METHOXYPHENOL.....	301(Vol 2)	C8H8O2	o-TOLUIC ACID.....	12(Vol 3)
C7H9N	BENZYLAMINE.....	302(Vol 2)	C8H8O2	p-TOLUIC ACID.....	13(Vol 3)
C7H9N	2,6-DIMETHYLPYRIDINE.....	303(Vol 2)	C8H8O3	METHYL SALICYLATE.....	14(Vol 3)
C7H9N	N-METHYLANILINE.....	304(Vol 2)	C8H8O3	VANILLIN.....	15(Vol 3)
C7H9N	m-TOLUIDINE.....	305(Vol 2)	C8H9NO	ACETANILIDE.....	16(Vol 3)
C7H9N	o-TOLUIDINE.....	306(Vol 2)	C8H10	ETHYLBENZENE.....	17(Vol 3)
C7H9N	p-TOLUIDINE.....	307(Vol 2)	C8H10	m-XYLENE.....	18(Vol 3)
C7H10	2-NORBORNENE.....	308(Vol 2)	C8H10	o-XYLENE.....	19(Vol 3)
C7H10N2	TOLUENEDIAMINE.....	309(Vol 2)	C8H10	p-XYLENE.....	20(Vol 3)
C7H11NO	CYCLOHEXYL ISOCYANATE.....	310(Vol 2)	C8H10O	m-ETHYLPHENOL.....	21(Vol 3)
C7H12O2	n-BUTYL ACRYLATE.....	311(Vol 2)	C8H10O	p-ETHYLPHENOL.....	22(Vol 3)
C7H12O2	ISOBUTYL ACRYLATE.....	312(Vol 2)	C8H10O	PHENETOLE.....	23(Vol 3)
C7H12O2	n-PROPYL METHACRYLATE.....	313(Vol 2)	C8H10O	2-PHENYLETHANOL.....	24(Vol 3)
C7H12O4	DIETHYL MALONATE.....	314(Vol 2)	C8H10O	2,3-XYLENOL.....	25(Vol 3)
C7H14	CYCLOHEPTANE.....	315(Vol 2)	C8H10O	2,4-XYLENOL.....	26(Vol 3)
C7H14	1,1-DIMETHYLCYCLOPENTANE.....	316(Vol 2)	C8H10O	2,5-XYLENOL.....	27(Vol 3)
C7H14	cis-1,2-DIMETHYLCYCLOPENTANE.....	317(Vol 2)	C8H10O	2,6-XYLENOL.....	28(Vol 3)
C7H14	trans-1,2-DIMETHYLCYCLOPENTANE.....	318(Vol 2)	C8H10O	3,4-XYLENOL.....	29(Vol 3)
C7H14	cis-1,3-DIMETHYLCYCLOPENTANE.....	319(Vol 2)	C8H10O	3,5-XYLENOL.....	30(Vol 3)
C7H14	trans-1,3-DIMETHYLCYCLOPENTANE.....	320(Vol 2)	C8H11N	N,N-DIMETHYLANILINE.....	31(Vol 3)
C7H14	ETHYLCYCLOPENTANE.....	321(Vol 2)	C8H11N	o-ETHYLANILINE.....	32(Vol 3)
C7H14	2-ETHYL-1-PENTENE.....	322(Vol 2)	C8H11N	2,4,6-TRIMETHYLPYRIDINE.....	33(Vol 3)
C7H14	3-ETHYL-1-PENTENE.....	323(Vol 2)	C8H11NO	p-PHENETIDINE.....	34(Vol 3)
C7H14	1-HEPTENE.....	324(Vol 2)	C8H12	1,5-CYCLOOCTADIENE.....	35(Vol 3)
C7H14	cis-2-HEPTENE.....	325(Vol 2)	C8H12	VINYLCYCLOHEXENE.....	36(Vol 3)
C7H14	trans-2-HEPTENE.....	326(Vol 2)	C8H12O4	1,4-CYCLOHEXANEDICARBOXYLIC ACID.....	37(Vol 3)
C7H14	cis-3-HEPTENE.....	327(Vol 2)	C8H12O4	DIETHYL MALEATE.....	38(Vol 3)
C7H14	trans-3-HEPTENE.....	328(Vol 2)	C8H14O2	n-BUTYL METHACRYLATE.....	39(Vol 3)
C7H14	METHYLCYCLOHEXANE.....	329(Vol 2)	C8H14O3	BUTYRIC ANHYDRIDE.....	40(Vol 3)
C7H14	2-METHYL-1-HEXENE.....	330(Vol 2)	C8H14O4	DIETHYL SUCCINATE.....	41(Vol 3)
C7H14	3-METHYL-1-HEXENE.....	331(Vol 2)	C8H16	1,1-DIMETHYLCYCLOHEXANE.....	42(Vol 3)
C7H14	4-METHYL-1-HEXENE.....	332(Vol 2)	C8H16	cis-1,2-DIMETHYLCYCLOHEXANE.....	43(Vol 3)
C7H14	2,3,3-TRIMETHYL-1-BUTENE.....	333(Vol 2)	C8H16	trans-1,2-DIMETHYLCYCLOHEXANE.....	44(Vol 3)
C7H14O	DIISOPROPYL KETONE.....	334(Vol 2)	C8H16	cis-1,3-DIMETHYLCYCLOHEXANE.....	45(Vol 3)
C7H14O	2-HEPTANONE.....	335(Vol 2)	C8H16	trans-1,3-DIMETHYLCYCLOHEXANE.....	46(Vol 3)
C7H14O	1-HEPTANAL.....	336(Vol 2)	C8H16	cis-1,4-DIMETHYLCYCLOHEXANE.....	47(Vol 3)
C7H14O	1-METHYLCYCLOHEXANOL.....	337(Vol 2)	C8H16	trans-1,4-DIMETHYLCYCLOHEXANE.....	48(Vol 3)
C7H14O	cis-2-METHYLCYCLOHEXANOL.....	338(Vol 2)	C8H16	ETHYLCYCLOHEXANE.....	49(Vol 3)
C7H14O	trans-2-METHYLCYCLOHEXANOL.....	339(Vol 2)	C8H16	2-ETHYL-1-HEXENE.....	50(Vol 3)
C7H14O	cis-3-METHYLCYCLOHEXANOL.....	340(Vol 2)	C8H16	1-METHYL-1-ETHYLCYCLOPENTANE.....	51(Vol 3)
C7H14O	trans-3-METHYLCYCLOHEXANOL.....	341(Vol 2)	C8H16	1-OCTENE.....	52(Vol 3)
C7H14O	cis-4-METHYLCYCLOHEXANOL.....	342(Vol 2)	C8H16	trans-2-OCTENE.....	53(Vol 3)
C7H14O	trans-4-METHYLCYCLOHEXANOL.....	343(Vol 2)	C8H16	trans-3-OCTENE.....	54(Vol 3)
C7H14O	5-METHYL-2-HEXANONE.....	344(Vol 2)	C8H16	trans-4-OCTENE.....	55(Vol 3)
C7H14O2	n-BUTYL PROPIONATE.....	345(Vol 2)	C8H16	n-PROPYLCYCLOPENTANE.....	56(Vol 3)
C7H14O2	ETHYL ISOVALERATE.....	346(Vol 2)	C8H16	2,4,4-TRIMETHYL-1-PENTENE.....	57(Vol 3)
C7H14O2	ISOPENTYL ACETATE.....	347(Vol 2)	C8H16	2,4,4-TRIMETHYL-2-PENTENE.....	58(Vol 3)
C7H14O2	n-PENTYL ACETATE.....	348(Vol 2)	C8H16O	2-ETHYLHEXANAL.....	59(Vol 3)
C7H14O2	n-PROPYL n-BUTYRATE.....	349(Vol 2)	C8H16O	1-OCTANAL.....	60(Vol 3)
C7H14O2	n-HEPTANOIC ACID.....	350(Vol 2)	C8H16O	2-OCTANONE.....	61(Vol 3)
C7H14O3	ETHYL-3-ETHOXYPROPIONATE.....	351(Vol 2)	C8H16O2	n-BUTYL n-BUTYRATE.....	62(Vol 3)
C7H15Br	1-BROMOHEPTANE.....	352(Vol 2)	C8H16O2	n-HEXYL ACETATE.....	63(Vol 3)
C7H15N	N-METHYLCYCLOHEXYLAMINE.....	353(Vol 2)	C8H16O2	ISOBUTYL ISOBUTYRATE.....	64(Vol 3)
C7H16	2,2-DIMETHYLPENTANE.....	354(Vol 2)	C8H16O2	n-OCTANOIC ACID.....	65(Vol 3)
C7H16	2,3-DIMETHYLPENTANE.....	355(Vol 2)	C8H16O4	DIETHYLENE GLYCOL ETHYL ETHER ACETATE.....	66(Vol 3)
C7H16	2,4-DIMETHYLPENTANE.....	356(Vol 2)	C8H18	2,2-DIMETHYLHEXANE.....	67(Vol 3)
C7H16	3,3-DIMETHYLPENTANE.....	357(Vol 2)	C8H18	2,3-DIMETHYLHEXANE.....	68(Vol 3)
C7H16	3-ETHYLPENTANE.....	358(Vol 2)	C8H18	2,4-DIMETHYLHEXANE.....	69(Vol 3)
C7H16	n-HEPTANE.....	359(Vol 2)	C8H18	2,5-DIMETHYLHEXANE.....	70(Vol 3)
C7H16	2-METHYLHEXANE.....	360(Vol 2)	C8H18	3,3-DIMETHYLHEXANE.....	71(Vol 3)
C7H16	3-METHYLHEXANE.....	361(Vol 2)	C8H18	3,4-DIMETHYLHEXANE.....	72(Vol 3)
C7H16	2,2,3-TRIMETHYLBUTANE.....	362(Vol 2)	C8H18	3-ETHYLHEXANE.....	73(Vol 3)
C7H16O	1-HEPTANOL.....	363(Vol 2)	C8H18	3-METHYL-3-ETHYLPENTANE.....	74(Vol 3)

C8H18	2-METHYLHEPTANE.....	75(Vol 3)	C9H20	2,2,5-TRIMETHYLHEXANE.....	153(Vol 3)
C8H18	3-METHYLHEPTANE.....	76(Vol 3)	C9H200	2,6-DIMETHYL-4-HEPTANOL.....	154(Vol 3)
C8H18	4-METHYLHEPTANE.....	77(Vol 3)	C9H200	1-NONANOL.....	155(Vol 3)
C8H18	n-OCTANE.....	78(Vol 3)	C9H200	2-NONANOL.....	156(Vol 3)
C8H18	2,2,3-TRIMETHYLPENTANE.....	79(Vol 3)	C9H20S	n-NONYL MERCAPTAN.....	157(Vol 3)
C8H18	2,2,4-TRIMETHYLPENTANE.....	80(Vol 3)	C9H21N	n-NONYLAMINE.....	158(Vol 3)
C8H18	2,3,3-TRIMETHYLPENTANE.....	81(Vol 3)	C9H21N	TRIPROPYLAMINE.....	159(Vol 3)
C8H18	2,3,4-TRIMETHYLPENTANE.....	82(Vol 3)	C10H608	PYROMELLITIC ACID.....	160(Vol 3)
C8H180	DI-n-BUTYL ETHER.....	83(Vol 3)	C10H7Br	1-BROMONAPHTHALENE.....	161(Vol 3)
C8H180	DI-sec-BUTYL ETHER.....	84(Vol 3)	C10H7Cl	1-CHLORONAPHTHALENE.....	162(Vol 3)
C8H180	DI-tert-BUTYL ETHER.....	85(Vol 3)	C10H8	NAPHTHALENE.....	163(Vol 3)
C8H180	2-ETHYL-1-HEXANOL.....	86(Vol 3)	C10H9N	QUINALDINE.....	164(Vol 3)
C8H180	1-OCTANOL.....	87(Vol 3)	C10H10	m-DIVINYLBENZENE.....	165(Vol 3)
C8H180	2-OCTANOL.....	88(Vol 3)	C10H10	1-METHYLINDENE.....	166(Vol 3)
C8H1802	DI-t-BUTYL PEROXIDE.....	89(Vol 3)	C10H10	2-METHYLINDENE.....	167(Vol 3)
C8H1802S	DI-n-BUTYL SULFONE.....	90(Vol 3)	C10H1004	OIMETHYL PHTHALATE.....	168(Vol 3)
C8H1803	DIETHYLENE GLYCOL DIETHYL ETHER.....	91(Vol 3)	C10H1004	DIMETHYL TEREPHTHALATE.....	169(Vol 3)
C8H1803	DIETHYLENE GLYCOL MONOBUTYL ETHER.....	92(Vol 3)	C10H12	OICYCLOPENTAOIENE.....	170(Vol 3)
C8H1804	TRIETHYLENE GLYCOL DIMETHYL ETHER.....	93(Vol 3)	C10H12	1,2,3,4-TETRAHYDRONAPHTHALENE.....	171(Vol 3)
C8H1805	TETRAETHYLENE GLYCOL.....	94(Vol 3)	C10H120	ANETHOLE.....	172(Vol 3)
C8H18S	n-OCTYL MERCAPTAN.....	95(Vol 3)	C10H1204	DIALLYL MALEATE.....	173(Vol 3)
C8H18S	tert-OCTYL MERCAPTAN.....	96(Vol 3)	C10H14	n-BUTYLBENZENE.....	174(Vol 3)
C8H19N	DI-n-BUTYLAMINE.....	97(Vol 3)	C10H14	sec-BUTYLBENZENE.....	175(Vol 3)
C8H19N	DIISOBUTYLAMINE.....	98(Vol 3)	C10H14	tert-BUTYLBENZENE.....	176(Vol 3)
C8H19N	n-OCTYLAMINE.....	99(Vol 3)	C10H14	m-CYMENE.....	177(Vol 3)
C8H23N5	TETRAETHYLENEPENTAMINE.....	100(Vol 3)	C10H14	o-CYMENE.....	178(Vol 3)
C8H24O4Si4	OCTAMETHYLCYCLOTETRASILLOXANE.....	101(Vol 3)	C10H14	p-CYMENE.....	179(Vol 3)
C9H405	TRIMELLITIC ANHYDRIDE.....	102(Vol 3)	C10H14	m-DIETHYLBENZENE.....	180(Vol 3)
C9H6N2O2	TOLUENE DIISOCYANATE.....	103(Vol 3)	C10H14	o-DIETHYLBENZENE.....	181(Vol 3)
C9H7N	ISOQUINOLINE.....	104(Vol 3)	C10H14	p-DIETHYLBENZENE.....	182(Vol 3)
C9H7N	QUINOLINE.....	105(Vol 3)	C10H14	2-ETHYL-m-XYLENE.....	183(Vol 3)
C9H7NO	8-HYDROXYQUINOLINE.....	106(Vol 3)	C10H14	2-ETHYL-p-XYLENE.....	184(Vol 3)
C9H8	INDENE.....	107(Vol 3)	C10H14	3-ETHYL-o-XYLENE.....	185(Vol 3)
C9H80	2-METHYLBENZOFURAN.....	108(Vol 3)	C10H14	4-ETHYL-m-XYLENE.....	186(Vol 3)
C9H10	INDANE.....	109(Vol 3)	C10H14	4-ETHYL-o-XYLENE.....	187(Vol 3)
C9H10	alpha-METHYLSTYRENE.....	110(Vol 3)	C10H14	5-ETHYL-m-XYLENE.....	188(Vol 3)
C9H10	m-METHYLSTYRENE.....	111(Vol 3)	C10H14	ISOBUTYLBENZENE.....	189(Vol 3)
C9H10	o-METHYLSTYRENE.....	112(Vol 3)	C10H14	1,2,3,5-TETRAMETHYLBENZENE.....	190(Vol 3)
C9H10	p-METHYLSTYRENE.....	113(Vol 3)	C10H14	1,2,4,5-TETRAMETHYLBENZENE.....	191(Vol 3)
C9H1002	BENZYL ACETATE.....	114(Vol 3)	C10H140	p-tert-BUTYLPHENOL.....	192(Vol 3)
C9H1002	ETHYL BENZOATE.....	115(Vol 3)	C10H1402	p-tert-BUTYLCATECHOL.....	193(Vol 3)
C9H1003	ETHYL VANILLIN.....	116(Vol 3)	C10H15N	N,N-DIETHYLANILINE.....	194(Vol 3)
C9H11NO	p-DIMETHYLAMINO BENZALDEHYDE.....	117(Vol 3)	C10H15N	2,6-DIETHYLANILINE.....	195(Vol 3)
C9H12	CUMENE.....	118(Vol 3)	C10H16	CAMPHENE.....	196(Vol 3)
C9H12	m-ETHYLTOLUENE.....	119(Vol 3)	C10H16	D-LIMONENE.....	197(Vol 3)
C9H12	o-ETHYLTOLUENE.....	120(Vol 3)	C10H16	alpha-PHELLANDRENE.....	198(Vol 3)
C9H12	p-ETHYLTOLUENE.....	121(Vol 3)	C10H16	beta-PHELLANDRENE.....	199(Vol 3)
C9H12	MESITYLENE.....	122(Vol 3)	C10H16	alpha-PINENE.....	200(Vol 3)
C9H12	n-PROPYLBENZENE.....	123(Vol 3)	C10H16	beta-PINENE.....	201(Vol 3)
C9H12	1,2,3-TRIMETHYLBENZENE.....	124(Vol 3)	C10H16	alpha-TERPINENE.....	202(Vol 3)
C9H12	1,2,4-TRIMETHYLBENZENE.....	125(Vol 3)	C10H16	gamma-TERPINENE.....	203(Vol 3)
C9H120	BENZYL ETHYL ETHER.....	126(Vol 3)	C10H16	TERPINOLENE.....	204(Vol 3)
C9H120	2-PHENYL-2-PROPANOL.....	127(Vol 3)	C10H160	CAMPHOR.....	205(Vol 3)
C9H1202	CUMENE HYDROPEROXIDE.....	128(Vol 3)	C10H18	cis-DECAHYDRONAPHTHALENE.....	206(Vol 3)
C9H140	ISOPHORONE.....	129(Vol 3)	C10H18	trans-DECAHYDRONAPHTHALENE.....	207(Vol 3)
C9H1406	GLYCERYL TRIACETATE.....	130(Vol 3)	C10H1804	SEBACIC ACID.....	208(Vol 3)
C9H1604	AZELAIC ACID.....	131(Vol 3)	C10H20	n-BUTYLCYCLOHEXANE.....	209(Vol 3)
C9H18	ISOPROPYLCYCLOHEXANE.....	132(Vol 3)	C10H20	1-DECENE.....	210(Vol 3)
C9H18	1-NONENE.....	133(Vol 3)	C10H200	1-DECANAL.....	211(Vol 3)
C9H18	n-PROPYLCYCLOHEXANE.....	134(Vol 3)	C10H2002	n-DECANOIC ACID.....	212(Vol 3)
C9H180	DIISOBUTYL KETONE.....	135(Vol 3)	C10H2002	2-ETHYLHEXYL ACETATE.....	213(Vol 3)
C9H180	1-NONANOL.....	136(Vol 3)	C10H2002	ISOPENTYL ISOVALERATE.....	214(Vol 3)
C9H1802	n-BUTYL VALERATE.....	137(Vol 3)	C10H22	n-DECANE.....	215(Vol 3)
C9H1802	n-NONANOIC ACID.....	138(Vol 3)	C10H22	2,2-DIMETHYLOCTANE.....	216(Vol 3)
C9H1802	n-OCTYL FORMATE.....	139(Vol 3)	C10H22	2-METHYLNONANE.....	217(Vol 3)
C9H20	3,3-DIETHYLPENTANE.....	140(Vol 3)	C10H22	3-METHYLNONANE.....	218(Vol 3)
C9H20	2,2-DIMETHYL-3-ETHYLPENTANE.....	141(Vol 3)	C10H22	4-METHYLNONANE.....	219(Vol 3)
C9H20	2,4-DIMETHYL-3-ETHYLPENTANE.....	142(Vol 3)	C10H22	5-METHYLNONANE.....	220(Vol 3)
C9H20	2,2-DIMETHYLHEPTANE.....	143(Vol 3)	C10H220	1-DECANOL.....	221(Vol 3)
C9H20	2,6-DIMETHYLHEPTANE.....	144(Vol 3)	C10H220	DI-n-PENTYL ETHER.....	222(Vol 3)
C9H20	3-ETHYLHEPTANE.....	145(Vol 3)	C10H220	ISODECANOL.....	223(Vol 3)
C9H20	2-METHYLOCTANE.....	146(Vol 3)	C10H2205	TETRAETHYLENE GLYCOL DIMETHYL ETHER.....	224(Vol 3)
C9H20	3-METHYLOCTANE.....	147(Vol 3)	C10H22S	n-DECYL MERCAPTAN.....	225(Vol 3)
C9H20	4-METHYLOCTANE.....	148(Vol 3)	C10H23N	n-DECYLAMINE.....	226(Vol 3)
C9H20	n-NONANE.....	149(Vol 3)	C11H10	1-METHYLNAPHTHALENE.....	227(Vol 3)
C9H20	2,2,3,3-TETRAMETHYLPENTANE.....	150(Vol 3)	C11H10	2-METHYLNAPHTHALENE.....	228(Vol 3)
C9H20	2,2,3,4-TETRAMETHYLPENTANE.....	151(Vol 3)	C11H1402	n-BUTYL BENZOATE.....	229(Vol 3)
C9H20	2,2,4,4-TETRAMETHYLPENTANE.....	152(Vol 3)	C11H16	n-PENTYLBENZENE.....	230(Vol 3)

C11H16O	p-tert-AMYLPHENOL.....	231(Vol 3)	C16H10	FLUORANTHENE.....	309(Vol 3)
C11H20O2	2-ETHYLHEXYL ACRYLATE.....	232(Vol 3)	C16H10	PYRENE.....	310(Vol 3)
C11H22	1-UNDECENE.....	233(Vol 3)	C16H12	1-PHENYLNAPHTHALENE.....	311(Vol 3)
C11H22O	1-UNDECANAL.....	234(Vol 3)	C16H20	1-n-HEXYLNAPHTHALENE.....	312(Vol 3)
C11H24	n-UNDECANE.....	235(Vol 3)	C16H22O4	DIBUTYL PHTHALATE.....	313(Vol 3)
C11H24O	1-UNDECANOL.....	236(Vol 3)	C16H26	n-DECYLBENZENE.....	314(Vol 3)
C11H24S	UNDECYL MERCAPTAN.....	237(Vol 3)	C16H32	n-DECYLCYCLOHEXANE.....	315(Vol 3)
C12H8O	DIBENZOFURAN.....	238(Vol 3)	C16H32	1-HEXADECENE.....	316(Vol 3)
C12H9N	DIBENZOPYRROLE.....	239(Vol 3)	C16H32O2	n-HEXADECANOIC ACID.....	317(Vol 3)
C12H10	ACENAPHTHENE.....	240(Vol 3)	C16H34	n-HEXADECANE.....	318(Vol 3)
C12H10	BIPHENYL.....	241(Vol 3)	C16H34O	DI-n-OCTYL ETHER.....	319(Vol 3)
C12H10O	DIPHENYL ETHER.....	242(Vol 3)	C16H34O	1-HEXADECANOL.....	320(Vol 3)
C12H11N	p-AMINODIPHENYL.....	243(Vol 3)	C17H28	n-UNDECYLBENZENE.....	321(Vol 3)
C12H11N	DIPHENYLAMINE.....	244(Vol 3)	C17H34	1-HEPTADECENE.....	322(Vol 3)
C12H11N3	p-AMINOAZOBENZENE.....	245(Vol 3)	C17H36	n-HEPTADECANE.....	323(Vol 3)
C12H11N3	1,3-DIPHENYLTRIAZENE.....	246(Vol 3)	C17H36O	1-HEPTADECANOL.....	324(Vol 3)
C12H12	2,6-DIMETHYLNAPHTHALENE.....	247(Vol 3)	C18H12	CHRYSENE.....	325(Vol 3)
C12H12	2,7-DIMETHYLNAPHTHALENE.....	248(Vol 3)	C18H14	m-TERPHENYL.....	326(Vol 3)
C12H12	1-ETHYLNAPHTHALENE.....	249(Vol 3)	C18H14	o-TERPHENYL.....	327(Vol 3)
C12H12N2	p-AMINODIPHENYLAMINE.....	250(Vol 3)	C18H14	p-TERPHENYL.....	328(Vol 3)
C12H12N2	HYDRAZOBENZENE.....	251(Vol 3)	C18H15P	TRIPHENYLPHOSPHINE.....	329(Vol 3)
C12H14	1,2,3-TRIMETHYLINDENE.....	252(Vol 3)	C18H15O4P	TRIPHENYL PHOSPHATE.....	330(Vol 3)
C12H14O4	DIETHYL PHTHALATE.....	253(Vol 3)	C18H16N2	N,N'-DIPHENYL-p-PHENYLENEDIAMINE.....	331(Vol 3)
C12H16	CYCLOHEXYLBENZENE.....	254(Vol 3)	C18H22	2,3-DIMETHYL-2,3-DIPHENYLBUTANE.....	332(Vol 3)
C12H18	m-DIISOPROPYLBENZENE.....	255(Vol 3)	C18H22O2	DICUMYL PEROXIDE.....	333(Vol 3)
C12H18	p-DIISOPROPYLBENZENE.....	256(Vol 3)	C18H30	n-DODECYLBENZENE.....	334(Vol 3)
C12H18	n-HEXYLBENZENE.....	257(Vol 3)	C18H32O2	LINOLEIC ACID.....	335(Vol 3)
C12H20O4	DIBUTYL MALEATE.....	258(Vol 3)	C18H34O2	OLEIC ACID.....	336(Vol 3)
C12H22	BICYCLOHEXYL.....	259(Vol 3)	C18H34O4	DIBUTYL SEBACATE.....	337(Vol 3)
C12H23N	DICYCLOHEXYLAMINE.....	260(Vol 3)	C18H34O4	DIHEXYL ADIPATE.....	338(Vol 3)
C12H24	1-DODECENE.....	261(Vol 3)	C18H36	1-OCTADECENE.....	339(Vol 3)
C12H24O	1-DODECANAL.....	262(Vol 3)	C18H36O2	STEARIC ACID.....	340(Vol 3)
C12H24O2	n-DODECANOIC ACID.....	263(Vol 3)	C18H38	n-OCTADECANE.....	341(Vol 3)
C12H26	n-DODECANE.....	264(Vol 3)	C18H38O	DINONYL ETHER.....	342(Vol 3)
C12H26O	DI-n-HEXYL ETHER.....	265(Vol 3)	C18H38O	1-OCTADECANOL.....	343(Vol 3)
C12H26O	1-DODECANOL.....	266(Vol 3)	C19H26	1-n-NONYLNAPHTHALENE.....	344(Vol 3)
C12H26O3	DIETHYLENE GLYCOL DI-n-BUTYL ETHER.....	267(Vol 3)	C19H32	n-TRIDECYLBENZENE.....	345(Vol 3)
C12H26S	n-DODECYL MERCAPTAN.....	268(Vol 3)	C19H36O2	METHYL OLEATE.....	346(Vol 3)
C12H27BO3	TRI-n-BUTYL BORATE.....	269(Vol 3)	C19H38	1-NONADECENE.....	347(Vol 3)
C12H27N	DODECYLAMINE.....	270(Vol 3)	C19H38O2	NONADECANOIC ACID.....	348(Vol 3)
C12H27N	TRI-n-BUTYLAMINE.....	271(Vol 3)	C19H40	n-NONADECANE.....	349(Vol 3)
C13H10	FLUORENE.....	272(Vol 3)	C20H16	TRIPHENYLETHYLENE.....	350(Vol 3)
C13H10O	BENZOPHENONE.....	273(Vol 3)	C20H28	1-n-DECYLNAPHTHALENE.....	351(Vol 3)
C13H12	DIPHENYLMETHANE.....	274(Vol 3)	C20H30O2	ABIETIC ACID.....	352(Vol 3)
C13H20	n-HEPTYLBENZENE.....	275(Vol 3)	C20H31N	DEHYDROABIETYLAMINE.....	353(Vol 3)
C13H26	1-TRIDECENE.....	276(Vol 3)	C20H40	1-EICOSENE.....	354(Vol 3)
C13H26O	1-TRIDECANAL.....	277(Vol 3)	C20H42	n-EICOSANE.....	355(Vol 3)
C13H26O2	n-BUTYL NONANOATE.....	278(Vol 3)	C20H42O	1-EICOSANOL.....	356(Vol 3)
C13H26O2	METHYL DODECANOATE.....	279(Vol 3)	C21H21O4P	TRI-o-CRESYL PHOSPHATE.....	357(Vol 3)
C13H28	n-TRIDECANE.....	280(Vol 3)	C22H44O2	n-BUTYL STEARATE.....	358(Vol 3)
C13H28O	1-TRIDECANOL.....	281(Vol 3)	C24H38O4	DIISOCTYL PHTHALATE.....	359(Vol 3)
C14H8O2	ANTHRAQUINONE.....	282(Vol 3)	C24H38O4	DIOCTYL PHTHALATE.....	360(Vol 3)
C14H10	ANTHRACENE.....	283(Vol 3)	C24H42O	DINONYLPHENOL.....	361(Vol 3)
C14H10	DIPHENYLACETYLENE.....	284(Vol 3)	C26H2O	TETRAPHENYLETHYLENE.....	362(Vol 3)
C14H10	PHENANTHRENE.....	285(Vol 3)	C28H46O4	DIISODECYL PHTHALATE.....	363(Vol 3)
C14H12	cis-STILBENE.....	286(Vol 3)			
C14H12	trans-STILBENE.....	287(Vol 3)			
C14H12O2	BENZYL BENZOATE.....	288(Vol 3)			
C14H14	1,1-DIPHENYLETHANE.....	289(Vol 3)			
C14H14	1,2-DIPHENYLETHANE.....	290(Vol 3)			
C14H14O	DIBENZYL ETHER.....	291(Vol 3)			
C14H16	1-n-BUTYLNAPHTHALENE.....	292(Vol 3)			
C14H22	n-OCTYLBENZENE.....	293(Vol 3)			
C14H22O	p-tert-OCTYLPHENOL.....	294(Vol 3)			
C14H28	1-TETRADECENE.....	295(Vol 3)			
C14H28O2	n-TETRADECANOIC ACID.....	296(Vol 3)			
C14H30	n-TETRADECANE.....	297(Vol 3)			
C14H30O	1-TETRADECANOL.....	298(Vol 3)			
C14H31N	TETRADECYLAMINE.....	299(Vol 3)			
C15H10N2O2	DIPHENYLMETHANE-4,4'-DIISOCYANATE.....	300(Vol 3)			
C15H16O	p-CUMYLPHENOL.....	301(Vol 3)			
C15H16O2	BISPHENOL A.....	302(Vol 3)			
C15H24	n-NONYLBENZENE.....	303(Vol 3)			
C15H24O	2,6-DI-tert-BUTYL-p-CRESOL.....	304(Vol 3)			
C15H24O	NONYLPHENOL.....	305(Vol 3)			
C15H30	1-PENTADECENE.....	306(Vol 3)			
C15H30O2	PENTADECANOIC ACID.....	307(Vol 3)			
C15H32	n-PENTADECANE.....	308(Vol 3)			

Appendix G

COMPOUND LIST BY NAME

ABIETIC ACID.....	352(Vol 3)	BROMOCHLOROMETHANE.....	19(Vol 1)
ACENAPHTHENE.....	240(Vol 3)	BROMOETHANE.....	106(Vol 1)
ACETAL.....	231(Vol 2)	1-BROMOHEPTANE.....	352(Vol 2)
ACETALDEHYDE.....	102(Vol 1)	1-BROMONAPHTHALENE.....	161(Vol 3)
ACETAMIDE.....	112(Vol 1)	1-BROMOPROPANE.....	177(Vol 1)
ACETANILIDE.....	16(Vol 3)	2-BROMOPROPANE.....	178(Vol 1)
ACETIC ACID.....	104(Vol 1)	p-BROMOTOLUENE.....	285(Vol 2)
ACETIC ANHYDRIDE.....	249(Vol 1)	BROMOTRICHLOROMETHANE.....	2(Vol 1)
ACETONE.....	164(Vol 1)	BROMOTRIFLUOROETHYLENE.....	45(Vol 1)
ACETONE CYANOHYDRIN.....	256(Vol 1)	BROMOTRIFLUOROMETHANE.....	3(Vol 1)
ACETONITRILE.....	92(Vol 1)	1,2-BUTADIENE.....	230(Vol 1)
ACETOPHENONE.....	9(Vol 3)	1,3-BUTADIENE.....	231(Vol 1)
ACETYL CHLORIDE.....	84(Vol 1)	n-BUTANE.....	290(Vol 1)
ACETYLLACETONE.....	28(Vol 2)	1,3-BUTANEOIOL.....	299(Vol 1)
ACETYLENE.....	66(Vol 1)	1,4-BUTANEOIOL.....	300(Vol 1)
ACROLEIN.....	141(Vol 1)	2,3-BUTANEDIOL.....	301(Vol 1)
ACRYLAMIDE.....	155(Vol 1)	n-BUTANOL.....	293(Vol 1)
ACRYLIC ACID.....	143(Vol 1)	sec-BUTANOL.....	294(Vol 1)
ACRYLONITRILE.....	136(Vol 1)	tert-BUTANOL.....	295(Vol 1)
ADIPIC ACID.....	165(Vol 2)	1-BUTENE.....	260(Vol 1)
ADIPONITRILE.....	140(Vol 2)	cis-2-BUTENE.....	261(Vol 1)
ALLYLAMINE.....	183(Vol 1)	trans-2-BUTENE.....	262(Vol 1)
ALLYL ACETATE.....	29(Vol 2)	cis-2-BUTENE-1,4-DIOL.....	272(Vol 1)
ALLYL ALCOHOL.....	165(Vol 1)	trans-2-BUTENE-1,4-DIOL.....	273(Vol 1)
p-AMINOAZOBENZENE.....	245(Vol 3)	2-BUTOXYETHANOL.....	232(Vol 2)
p-AMINODIPHENYL.....	243(Vol 3)	n-BUTYL ACETATE.....	199(Vol 2)
p-AMINODIPHENYLAMINE.....	250(Vol 3)	sec-BUTYL ACETATE.....	200(Vol 2)
2-AMINOETHOXYETHANOL.....	321(Vol 1)	tert-BUTYL ACETATE.....	201(Vol 2)
N-AMINOETHYL ETHANOLAMINE.....	320(Vol 1)	n-BUTYL ACRYLATE.....	311(Vol 2)
N-AMINOETHYL PIPERAZINE.....	252(Vol 2)	n-BUTYL BENZOATE.....	229(Vol 3)
1-AMINOHEPTANE.....	367(Vol 2)	n-BUTYL n-BUTYRATE.....	62(Vol 3)
6-AMINOHEXANOL.....	249(Vol 2)	n-BUTYL CHLORIDE.....	284(Vol 1)
1-AMINO-2-PROPANOL.....	203(Vol 1)	sec-BUTYL CHLORIDE.....	285(Vol 1)
3-AMINO-1-PROPANOL.....	204(Vol 1)	tert-BUTYL CHLORIDE.....	286(Vol 1)
p-tert-AMYLPHENOL.....	231(Vol 3)	n-BUTYL ETHYL ETHER.....	227(Vol 2)
ANETHOLE.....	172(Vol 3)	n-BUTYL FORMATE.....	53(Vol 2)
ANILINE.....	134(Vol 2)	sec-BUTYL GLYCOLATE.....	213(Vol 2)
ANISOLE.....	295(Vol 2)	t-BUTYL HYDROPEROXIDE.....	302(Vol 1)
ANTHRACENE.....	283(Vol 3)	n-BUTYL ISOCYANATE.....	38(Vol 2)
ANTHRAQUINONE.....	282(Vol 3)	n-BUTYL MERCAPTAN.....	307(Vol 1)
ASCORBIC ACID.....	148(Vol 2)	sec-BUTYL MERCAPTAN.....	309(Vol 1)
AZELAIC ACID.....	131(Vol 3)	tert-BUTYL MERCAPTAN.....	310(Vol 1)
BENZALDEHYDE.....	280(Vol 2)	n-BUTYL METHACRYLATE.....	39(Vol 3)
BENZENE.....	118(Vol 2)	n-BUTYL NONANOATE.....	278(Vol 3)
1,2-BENZENEDIOL.....	129(Vol 2)	n-BUTYL PROPIONATE.....	345(Vol 2)
1,3-BENZENEDIOL.....	130(Vol 2)	n-BUTYL STEARATE.....	358(Vol 3)
1,2,3-BENZENETRIOL.....	132(Vol 2)	n-BUTYL VALERATE.....	137(Vol 3)
BENZOIC ACID.....	281(Vol 2)	BUTYL VINYL ETHER.....	191(Vol 2)
BENZONITRILE.....	270(Vol 2)	n-BUTYLAMINE.....	313(Vol 1)
BENZOPHENONE.....	273(Vol 3)	sec-BUTYLAMINE.....	315(Vol 1)
BENZOTHIOPHENE.....	6(Vol 3)	tert-BUTYLAMINE.....	316(Vol 1)
BENZOTRICHLORIDE.....	268(Vol 2)	n-BUTYLBENZENE.....	174(Vol 3)
BENZOTRIFLUORIDE.....	269(Vol 2)	sec-BUTYLBENZENE.....	175(Vol 3)
BENZOYL CHLORIDE.....	266(Vol 2)	tert-BUTYLBENZENE.....	176(Vol 3)
BENZYL ACETATE.....	114(Vol 3)	p-tert-BUTYLCATECHOL.....	193(Vol 3)
BENZYL ALCOHOL.....	296(Vol 2)	n-BUTYLCYCLOHEXANE.....	209(Vol 3)
BENZYL BENZOATE.....	288(Vol 3)	tert-BUTYLFORMAMIOE.....	69(Vol 2)
BENZYL CHLORIDE.....	286(Vol 2)	1-n-BUTYLNAPHTHALENE.....	292(Vol 3)
BENZYL DICHLORIDE.....	273(Vol 2)	p-tert-BUTYLPHENOL.....	192(Vol 3)
BENZYL ETHYL ETHER.....	126(Vol 3)	2-BUTYNE-1,4-DIOL.....	242(Vol 1)
BENZYLAMINE.....	302(Vol 2)	n-BUTYRALDEHYDE.....	266(Vol 1)
BICYCLOHEXYL.....	259(Vol 3)	n-BUTYRIC ACID.....	275(Vol 1)
BIPHENYL.....	241(Vol 3)	BUTYRIC ANHYDRIDE.....	40(Vol 3)
BIS(CHLOROMETHYL)ETHER.....	99(Vol 1)	gamma-BUTYROLACTONE.....	243(Vol 1)
BIS(CYANOETHYL)ETHER.....	146(Vol 2)	n-BUTYRONITRILE.....	254(Vol 1)
BISPHENOL A.....	302(Vol 3)	CAMPHENE.....	196(Vol 3)
BROMOBENZENE.....	109(Vol 2)	CAMPHOR.....	205(Vol 3)
1-BROMOBUTANE.....	282(Vol 1)	epsilon-CAPROLACTAM.....	170(Vol 2)
2-BROMOBUTANE.....	283(Vol 1)	epsilon-CAPROLACTONE.....	160(Vol 2)
BROMOCHLORODIFLUOROMETHANE.....	1(Vol 1)	CARBON DIOXIDE.....	44(Vol 1)

CARBON DISULFIDE.....	48(Vol 1)
CARBON MONOXIDE.....	42(Vol 1)
CARBON TETRACHLORIDE.....	10(Vol 1)
CARBON TETRAFLUORIDE.....	12(Vol 1)
CARBONYL FLUORIDE.....	11(Vol 1)
CARBONYL SULFIDE.....	43(Vol 1)
CHLOROACETALDEHYDE.....	85(Vol 1)
CHLOROACETIC ACID.....	86(Vol 1)
CHLOROACETYL CHLORIDE.....	71(Vol 1)
o-CHLOROANILINE.....	120(Vol 2)
m-CHLOROANILINE.....	119(Vol 2)
p-CHLOROANILINE.....	121(Vol 2)
o-CHLOROBENZOIC ACID.....	267(Vol 2)
p-CHLOROBENZOTRIFLUORIDE.....	263(Vol 2)
m-CHLOROBENZOYL CHLORIDE.....	264(Vol 2)
1-CHLORO-1,1-DIFLUOROETHANE.....	83(Vol 1)
2-CHLORO-1,1-DIFLUOROETHYLENE.....	59(Vol 1)
CHLORODIFLUOROMETHANE.....	14(Vol 1)
1-CHLORO-2,4-DINITROBENZENE.....	95(Vol 2)
2-CHLOROETHANOL.....	108(Vol 1)
CHLOROFORM.....	16(Vol 1)
1-CHLORONAPHTHALENE.....	162(Vol 3)
o-CHLORONITROBENZENE.....	101(Vol 2)
m-CHLORONITROBENZENE.....	100(Vol 2)
p-CHLORONITROBENZENE.....	102(Vol 2)
4-CHLORO-3-NITROBENZOTRIFLUORIDE.....	260(Vol 2)
CHLOROPENTAFLUOROETHANE.....	49(Vol 1)
1-CHLOROPENTANE.....	66(Vol 2)
o-CHLOROPHENOL.....	112(Vol 2)
m-CHLOROPHENOL.....	111(Vol 2)
p-CHLOROPHENOL.....	113(Vol 2)
CHLOROPRENE.....	223(Vol 1)
2-CHLOROPROPENE.....	148(Vol 1)
3-CHLOROPROPENE.....	149(Vol 1)
o-CHLOROTOLUENE.....	287(Vol 2)
p-CHLOROTOLUENE.....	288(Vol 2)
CHLOROTRIFLUOROETHYLENE.....	47(Vol 1)
CHLOROTRIFLUOROMETHANE.....	5(Vol 1)
CHRYSENE.....	325(Vol 3)
CITRACONIC ACID.....	11(Vol 2)
CITRIC ACID.....	149(Vol 2)
m-CRESOL.....	297(Vol 2)
o-CRESOL.....	298(Vol 2)
p-CRESOL.....	299(Vol 2)
trans-CROTONALDEHYDE.....	238(Vol 1)
cis-CROTONIC ACID.....	244(Vol 1)
trans-CROTONIC ACID.....	245(Vol 1)
trans-CROTONITRILE.....	224(Vol 1)
cis-CROTONITRILE.....	225(Vol 1)
CUMENE.....	118(Vol 3)
CUMENE HYDROPEROXIDE.....	128(Vol 3)
p-CUMYLPHENOL.....	301(Vol 3)
CYANOGEN.....	130(Vol 1)
CYANOGEN CHLORIDE.....	6(Vol 1)
CYCLOBUTANE.....	263(Vol 1)
CYCLOHEPTANE.....	315(Vol 2)
1,3-CYCLOHEXADIENE.....	138(Vol 2)
CYCLOHEXANE.....	172(Vol 2)
1,4-CYCLOHEXANEDICARBOXYLIC ACID.....	37(Vol 3)
CYCLOHEXANOL.....	192(Vol 2)
CYCLOHEXANONE.....	158(Vol 2)
CYCLOHEXANONE OXIME.....	171(Vol 2)
CYCLOHEXENE.....	150(Vol 2)
CYCLOHEXYL ISOCYANATE.....	310(Vol 2)
CYCLOHEXYL PEROXIDE.....	206(Vol 2)
CYCLOHEXYLAMINE.....	214(Vol 2)
CYCLOHEXYLBENZENE.....	254(Vol 3)
1,5-CYCLOOCTADIENE.....	35(Vol 3)
CYCLOPENTADIENE.....	4(Vol 2)
CYCLOPENTANE.....	41(Vol 2)
CYCLOPENTANONE.....	26(Vol 2)
CYCLOPENTENE.....	15(Vol 2)
CYCLOPROPANE.....	159(Vol 1)
m-CYMENE.....	177(Vol 3)
o-CYMENE.....	178(Vol 3)
p-CYMENE.....	179(Vol 3)
DECAFLUOROBUTANE.....	213(Vol 1)
1-DECANAL.....	211(Vol 3)

n-DECANE.....	215(Vol 3)
n-DECANOIC ACID.....	212(Vol 3)
1-DECANOL.....	221(Vol 3)
1-DECENE.....	210(Vol 3)
n-DECYL MERCAPTAN.....	225(Vol 3)
n-DECYLAMINE.....	226(Vol 3)
n-DECYLBENZENE.....	314(Vol 3)
n-DECYLCYCLOHEXANE.....	315(Vol 3)
1-n-DECYLNAPHTHALENE.....	351(Vol 3)
DEHYDROABIETYLAMINE.....	353(Vol 3)
cis-DECAHYDRONAPHTHALENE.....	206(Vol 3)
trans-DECAHYDRONAPHTHALENE.....	207(Vol 3)
DIACETONE ALCOHOL.....	207(Vol 2)
DIALLYL MALEATE.....	173(Vol 3)
DIBENZOFURAN.....	238(Vol 3)
DIBENZOPYRROLE.....	239(Vol 3)
DIBENZYL ETHER.....	291(Vol 3)
m-DIBROMOBENZENE.....	99(Vol 2)
DIBROMODIFLUOROMETHANE.....	4(Vol 1)
1,1-DIBROMOETHANE.....	95(Vol 1)
1,2-DIBROMOETHANE.....	96(Vol 1)
DIBROMOMETHANE.....	20(Vol 1)
1,2-DIBROMOTETRAFLUOROETHANE.....	46(Vol 1)
DI-n-BUTYL ETHER.....	83(Vol 3)
DI-sec-BUTYL ETHER.....	84(Vol 3)
DI-tert-BUTYL ETHER.....	85(Vol 3)
DIBUTYL MALEATE.....	258(Vol 3)
DI-n-BUTYL SULFONE.....	90(Vol 3)
DI-t-BUTYL PEROXIDE.....	89(Vol 3)
DIBUTYL PHTHALATE.....	313(Vol 3)
DIBUTYL SEBACATE.....	337(Vol 3)
DI-n-BUTYLAMINE.....	97(Vol 3)
2,6-DI-tert-BUTYL-p-CRESOL.....	304(Vol 3)
DICHLOROACETALDEHYDE.....	72(Vol 1)
DICHLOROACETIC ACID.....	73(Vol 1)
DICHLOROACETYL CHLORIDE.....	61(Vol 1)
3,4-DICHLOROANILINE.....	114(Vol 2)
m-DICHLOROBENZENE.....	103(Vol 2)
o-DICHLOROBENZENE.....	104(Vol 2)
p-DICHLOROBENZENE.....	105(Vol 2)
2,4-DICHLOROBENZOTRIFLUORIDE.....	261(Vol 2)
1,4-DICHLOROBUTANE.....	265(Vol 1)
1,3-DICHLORO-trans-2-BUTENE.....	234(Vol 1)
1,4-DICHLORO-cis-2-BUTENE.....	235(Vol 1)
1,4-DICHLORO-trans-2-BUTENE.....	236(Vol 1)
3,4-DICHLORO-1-BUTENE.....	237(Vol 1)
DICHLORODIFLUOROMETHANE.....	7(Vol 1)
1,1-DICHLOROETHANE.....	97(Vol 1)
1,2-DICHLOROETHANE.....	98(Vol 1)
1,1-DICHLOROETHYLENE.....	68(Vol 1)
cis-1,2-DICHLOROETHYLENE.....	69(Vol 1)
trans-1,2-DICHLOROETHYLENE.....	70(Vol 1)
DICHLOROFUOROMETHANE.....	15(Vol 1)
DICHLOROMETHANE.....	21(Vol 1)
1,2-DICHLORO-4-NITROBENZENE.....	96(Vol 2)
1,5-DICHLOROPENTANE.....	48(Vol 2)
3,4-DICHLOROPHENYL ISOCYANATE.....	262(Vol 2)
1,1-DICHLOROPROPANE.....	161(Vol 1)
1,2-DICHLOROPROPANE.....	162(Vol 1)
1,3-DICHLOROPROPANE.....	163(Vol 2)
2,3-DICHLOROPROPENE.....	140(Vol 1)
1,2-DICHLOROTETRAFLUOROETHANE.....	50(Vol 1)
2,4-DICHLOROTOLUENE.....	274(Vol 2)
DICUMYL PEROXIDE.....	333(Vol 3)
1,4-DICYANO-2-BUTENE.....	124(Vol 2)
cis-DICYANO-1-BUTENE.....	122(Vol 2)
trans-DICYANO-1-BUTENE.....	123(Vol 2)
DICYCLOHEXYLAMINE.....	260(Vol 3)
DICYCLOPENTADIENE.....	170(Vol 3)
DIETHANOLAMINE.....	319(Vol 1)
DIETHYL CARBONATE.....	64(Vol 2)
DIETHYL DISULFIDE.....	312(Vol 1)
DIETHYL ETHER.....	296(Vol 1)
DIETHYL KETONE.....	51(Vol 2)
DIETHYL MALEATE.....	38(Vol 3)
DIETHYL MALONATE.....	314(Vol 2)
DIETHYL OXALATE.....	166(Vol 2)
DIETHYL PHTHALATE.....	253(Vol 3)

DIETHYL SUCCINATE.....	41(Vol 3)
DIETHYL SULFATE.....	306(Vol 1)
DIETHYL SULFIDE.....	311(Vol 1)
DIETHYLAMINE.....	317(Vol 1)
N,N-DIETHYLANILINE.....	194(Vol 3)
2,6-DIETHYLANILINE.....	195(Vol 3)
o-DIETHYLBENZENE.....	181(Vol 3)
m-DIETHYLBENZENE.....	180(Vol 3)
p-DIETHYLBENZENE.....	182(Vol 3)
DIETHYLENE GLYCOL.....	305(Vol 1)
DIETHYLENE GLYCOL DI-n-BUTYL ETHER.....	267(Vol 3)
DIETHYLENE GLYCOL DIETHYL ETHER.....	91(Vol 3)
DIETHYLENE GLYCOL DIMETHYL ETHER.....	236(Vol 2)
DIETHYLENE GLYCOL ETHYL ETHER ACETATE.....	66(Vol 3)
DIETHYLENE GLYCOL MONOBUTYL ETHER.....	92(Vol 3)
DIETHYLENE TRIAMINE.....	323(Vol 1)
3,3-DIETHYLPENTANE.....	140(Vol 3)
1,1-DIFLUOROETHANE.....	100(Vol 1)
1,2-DIFLUOROETHANE.....	101(Vol 1)
1,1-DIFLUOROETHYLENE.....	77(Vol 1)
DIFLUOROMETHANE.....	22(Vol 1)
DIGLYCOLIC ACID.....	251(Vol 1)
DIHEXYL ADIPATE.....	338(Vol 3)
DI-n-HEXYL ETHER.....	265(Vol 3)
2,5-DIHYDROFURAN.....	239(Vol 1)
DIIODOMETHANE.....	23(Vol 1)
DIISOBUTYL KETONE.....	135(Vol 3)
DIISOBUTYLAMINE.....	98(Vol 3)
DIISODECYL PHTHALATE.....	363(Vol 3)
DIISOPROPANOLAMINE.....	250(Vol 2)
DIISOPROPYL ETHER.....	228(Vol 2)
DIISOPROPYL KETONE.....	334(Vol 2)
DIISOPROPYLAMINE.....	245(Vol 2)
m-DIISOPROPYLBENZENE.....	255(Vol 3)
p-DIISOPROPYLBENZENE.....	256(Vol 3)
DIISOCTYL PHTHALATE.....	359(Vol 3)
DIKETENE.....	218(Vol 1)
1,2-DIMETHOXYETHANE.....	303(Vol 1)
DIMETHYL DISULFIDE.....	124(Vol 1)
DIMETHYL ETHER.....	117(Vol 1)
DIMETHYL MALEATE.....	147(Vol 2)
DIMETHYL PHTHALATE.....	168(Vol 3)
DIMETHYL SILANE.....	129(Vol 1)
DIMETHYL SULFATE.....	121(Vol 1)
DIMETHYL SULFIDE.....	122(Vol 1)
DIMETHYL SULFOXIDE.....	119(Vol 1)
DIMETHYL TEREPHTHALATE.....	169(Vol 3)
N,N-DIMETHYLACETAMIDE.....	288(Vol 1)
DIMETHYLACETYLENE.....	232(Vol 1)
DIMETHYALUMINUM CHLORIDE.....	116(Vol 1)
DIMETHYLAMINE.....	125(Vol 1)
p-DIMETHYLAMINO BENZALDEHYDE.....	117(Vol 3)
N,N-DIMETHYLANILINE.....	31(Vol 3)
2,3-DIMETHYL-1,3-BUTADIENE.....	151(Vol 2)
2,2-DIMETHYLBUTANE.....	216(Vol 2)
2,3-DIMETHYLBUTANE.....	217(Vol 2)
2,3-DIMETHYL-1-BUTENE.....	173(Vol 2)
2,3-DIMETHYL-2-BUTENE.....	174(Vol 2)
3,3-DIMETHYL-1-BUTENE.....	175(Vol 2)
1,1-DIMETHYLCYCLOHEXANE.....	42(Vol 3)
cis-1,2-DIMETHYLCYCLOHEXANE.....	43(Vol 3)
cis-1,3-DIMETHYLCYCLOHEXANE.....	45(Vol 3)
cis-1,4-DIMETHYLCYCLOHEXANE.....	47(Vol 3)
trans-1,2-DIMETHYLCYCLOHEXANE.....	44(Vol 3)
trans-1,3-DIMETHYLCYCLOHEXANE.....	46(Vol 3)
trans-1,4-DIMETHYLCYCLOHEXANE.....	48(Vol 3)
1,1-DIMETHYLCYCLOPENTANE.....	316(Vol 2)
cis-1,2-DIMETHYLCYCLOPENTANE.....	317(Vol 2)
trans-1,2-DIMETHYLCYCLOPENTANE.....	318(Vol 2)
cis-1,3-DIMETHYLCYCLOPENTANE.....	319(Vol 2)
trans-1,3-DIMETHYLCYCLOPENTANE.....	320(Vol 2)
2,3-DIMETHYL-2,3-DIPHENYLBUTANE.....	332(Vol 3)
DIMETHYLETHANOLAMINE.....	318(Vol 1)
2,2-DIMETHYL-3-ETHYLPENTANE.....	141(Vol 3)
2,4-DIMETHYL-3-ETHYLPENTANE.....	142(Vol 3)
N,N-DIMETHYLFORMAMIDE.....	185(Vol 1)
2,2-DIMETHYLHEPTANE.....	143(Vol 3)
2,6-DIMETHYLHEPTANE.....	144(Vol 3)

2,6-DIMETHYL-4-HEPTANOL.....	154(Vol 3)
2,2-DIMETHYLHEXANE.....	67(Vol 3)
2,3-DIMETHYLHEXANE.....	68(Vol 3)
2,4-DIMETHYLHEXANE.....	69(Vol 3)
2,5-DIMETHYLHEXANE.....	70(Vol 3)
3,3-DIMETHYLHEXANE.....	71(Vol 3)
3,4-DIMETHYLHEXANE.....	72(Vol 3)
2,6-DIMETHYLNAPHTHALENE.....	247(Vol 3)
2,7-DIMETHYLNAPHTHALENE.....	248(Vol 3)
2,2-DIMETHYLOCTANE.....	216(Vol 3)
2,2-DIMETHYLPENTANE.....	354(Vol 2)
2,3-DIMETHYLPENTANE.....	355(Vol 2)
2,4-DIMETHYLPENTANE.....	356(Vol 2)
3,3-DIMETHYLPENTANE.....	357(Vol 2)
2,2-DIMETHYL-1-PROPANOL.....	73(Vol 2)
2,6-DIMETHYLPYRIDINE.....	303(Vol 2)
m-DINITROBENZENE.....	106(Vol 2)
o-DINITROBENZENE.....	107(Vol 2)
p-DINITROBENZENE.....	108(Vol 2)
2,5-DINITROTOLUENE.....	276(Vol 2)
2,4-DINITROTOLUENE.....	275(Vol 2)
2,6-DINITROTOLUENE.....	277(Vol 2)
3,5-DINITROTOLUENE.....	279(Vol 2)
3,4-DINITROTOLUENE.....	278(Vol 2)
DINONYL ETHER.....	342(Vol 3)
DINONYLPHENOL.....	361(Vol 3)
DI-n-OCTYL ETHER.....	319(Vol 3)
DIOCTYL PHTHALATE.....	360(Vol 3)
1,4-DIOXANE.....	276(Vol 1)
DI-n-PENTYL ETHER.....	222(Vol 3)
DIPHENYL ETHER.....	242(Vol 3)
DIPHENYLACETYLENE.....	284(Vol 3)
DIPHENYLAMINE.....	244(Vol 3)
1,1-DIPHENYLETHANE.....	289(Vol 3)
1,2-DIPHENYLETHANE.....	290(Vol 3)
DIPHENYLMETHANE-4,4'-DIISOCYANATE.....	300(Vol 3)
N,N'-DIPHENYL-p-PHENYLENEDIAMINE.....	331(Vol 3)
1,3-DIPHENYLTIAZENE.....	246(Vol 3)
DIPHENYLMETHANE.....	274(Vol 3)
DI-n-PROPYL ETHER.....	229(Vol 2)
DI-n-PROPYL SULFONE.....	235(Vol 2)
DI-n-PROPYLAMINE.....	246(Vol 2)
DIPROPYLENE GLYCOL.....	237(Vol 2)
DIVINYL ETHER.....	240(Vol 1)
m-DIVINYLBENZENE.....	165(Vol 3)
1-DODECANAL.....	262(Vol 3)
n-DODECANE.....	264(Vol 3)
n-DODECANOIC ACID.....	263(Vol 3)
1-DODECANOL.....	266(Vol 3)
1-DODECENE.....	261(Vol 3)
n-DODECYL MERCAPTAN.....	268(Vol 3)
DODECYLAMINE.....	270(Vol 3)
n-DODECYLBENZENE.....	334(Vol 3)
n-EICOSANE.....	355(Vol 3)
1-EICOSANOL.....	356(Vol 3)
1-EICOSENE.....	354(Vol 3)
alpha-EPICHLOROHYDRIN.....	150(Vol 1)
1,2-EPOXYBUTANE.....	268(Vol 1)
ETHANE.....	115(Vol 1)
ETHANOL.....	118(Vol 1)
2-ETHOXYETHANOL.....	304(Vol 1)
2-(2-ETHOXYETHOXY)ETHANOL.....	238(Vol 2)
2-ETHOXYETHYL ACETATE.....	210(Vol 2)
ETHYL ACETATE.....	277(Vol 1)
ETHYL ACRYLATE.....	30(Vol 2)
ETHYL ALUMINUM SESQUICHLORIDE.....	244(Vol 2)
ETHYL BENZOATE.....	115(Vol 3)
ETHYL n-BUTYRATE.....	202(Vol 2)
2-ETHYL BUTYRIC ACID.....	208(Vol 2)
ETHYL CHLORIDE.....	107(Vol 1)
ETHYL CHLOROFORMATE.....	152(Vol 1)
ETHYL CYANOACETATE.....	14(Vol 2)
ETHYL FLUORIDE.....	109(Vol 1)
ETHYL FORMATE.....	170(Vol 1)
ETHYL IODIDE.....	110(Vol 1)
ETHYL ISOBUTYRATE.....	203(Vol 2)
ETHYL ISOPROPYL KETONE.....	194(Vol 2)
ETHYL ISOVALERATE.....	346(Vol 2)

ETHYL LACTATE.....	65(Vol 2)	cis-3-HEPTENE.....	327(Vol 2)
ETHYL MERCAPTAN.....	123(Vol 1)	trans-2-HEPTENE.....	326(Vol 2)
ETHYL METHACRYLATE.....	161(Vol 2)	trans-3-HEPTENE.....	328(Vol 2)
ETHYL PROPIONATE.....	54(Vol 2)	n-HEPTYL MERCAPTAN.....	366(Vol 2)
ETHYL PROPYL ETHER.....	84(Vol 2)	n-HEPTYLBENZENE.....	275(Vol 3)
ETHYL VANILLIN.....	116(Vol 3)	HEXACHLORO BENZENE.....	93(Vol 2)
ETHYL VINYL ETHER.....	270(Vol 1)	HEXACHLORO-1,3-BUTADIENE.....	210(Vol 1)
ETHYLACETOACETATE.....	163(Vol 2)	HEXACHLOROCYCLOPENTADIENE.....	1(Vol 2)
ETHYLACETYLENE.....	233(Vol 1)	HEXACHLOROETHANE.....	55(Vol 1)
ETHYLAMINE.....	126(Vol 1)	n-HEXADECANE.....	318(Vol 3)
o-ETHYLANILINE.....	32(Vol 3)	n-HEXADECANOIC ACID.....	317(Vol 3)
ETHYLBENZENE.....	17(Vol 3)	1-HEXADECANOL.....	320(Vol 3)
2-ETHYL-1-BUTENE.....	176(Vol 2)	1-HEXADECENE.....	316(Vol 3)
2-ETHYL-1-BUTANOL.....	222(Vol 2)	1,5-HEXADIENE.....	152(Vol 2)
ETHYLCYCLOHEXANE.....	49(Vol 3)	cis,trans-2,4-HEXADIENE.....	153(Vol 2)
ETHYLCYCLOPENTANE.....	321(Vol 2)	trans,trans-2,4-HEXADIENE.....	154(Vol 2)
ETHYLENE.....	94(Vol 1)	HEXAFLUOROACETONE.....	132(Vol 1)
ETHYLENE CARBONATE.....	146(Vol 1)	HEXAFLUOROBENZENE.....	94(Vol 2)
ETHYLENE GLYCOL.....	120(Vol 1)	HEXAFLUOROETHANE.....	57(Vol 1)
ETHYLENE GLYCOL DIACETATE.....	167(Vol 2)	HEXAFLUOROPROPYLENE.....	131(Vol 1)
ETHYLENE GLYCOL MONOPROPYL ETHER.....	85(Vol 2)	HEXAMETHYL PHOSPHORAMIDE.....	255(Vol 2)
ETHYLENE OXIDE.....	103(Vol 1)	HEXAMETHYLCYCLOTRISILOXANE.....	258(Vol 2)
ETHYLENEDIAMINE.....	128(Vol 1)	HEXAMETHYLDISILAZANE.....	259(Vol 2)
ETHYLENEIMINE.....	111(Vol 1)	HEXAMETHYLDISILOXANE.....	257(Vol 2)
ETHYL-3-ETHOXYPROPIONATE.....	351(Vol 2)	HEXAMETHYLENEDIAMINE.....	254(Vol 2)
3-ETHYLHEPTANE.....	145(Vol 3)	HEXAMETHYLENEIMINE.....	215(Vol 2)
2-ETHYLHEXANAL.....	59(Vol 3)	1-HEXANAL.....	193(Vol 2)
3-ETHYLHEXANE.....	73(Vol 3)	n-HEXANE.....	218(Vol 2)
2-ETHYL-1-HEXANOL.....	86(Vol 3)	1,6-HEXANEDIOL.....	233(Vol 2)
2-ETHYL-1-HEXENE.....	50(Vol 3)	HEXANENITRILE.....	169(Vol 2)
2-ETHYLHEXYL ACETATE.....	213(Vol 3)	n-HEXANOIC ACID.....	209(Vol 2)
2-ETHYLHEXYL ACRYLATE.....	232(Vol 3)	1-HEXANOL.....	223(Vol 2)
ETHYLIDENE DIACETATE.....	168(Vol 2)	2-HEXANOL.....	224(Vol 2)
1-ETHYLNAPHTHALENE.....	249(Vol 3)	2-HEXANONE.....	195(Vol 2)
3-ETHYLPENTANE.....	358(Vol 2)	3-HEXANONE.....	196(Vol 2)
2-ETHYL-1-PENTENE.....	322(Vol 2)	1-HEXENE.....	177(Vol 2)
3-ETHYL-1-PENTENE.....	323(Vol 2)	cis-2-HEXENE.....	178(Vol 2)
m-ETHYLPHENOL.....	21(Vol 3)	cis-3-HEXENE.....	180(Vol 2)
p-ETHYLPHENOL.....	22(Vol 3)	trans-2-HEXENE.....	179(Vol 2)
m-ETHYLTOLUENE.....	119(Vol 3)	trans-3-HEXENE.....	181(Vol 2)
o-ETHYLTOLUENE.....	120(Vol 3)	n-HEXYL ACETATE.....	63(Vol 3)
p-ETHYLTOLUENE.....	121(Vol 3)	n-HEXYLAMINE.....	247(Vol 2)
2-ETHYL-m-XYLENE.....	183(Vol 3)	n-HEXYLBENZENE.....	257(Vol 3)
2-ETHYL-p-XYLENE.....	184(Vol 3)	HEXYLENE GLYCOL.....	234(Vol 2)
3-ETHYL-o-XYLENE.....	185(Vol 3)	n-HEXYLMERCAPTAN.....	242(Vol 2)
4-ETHYL-m-XYLENE.....	186(Vol 3)	1-n-HEXYLNAPHTHALENE.....	312(Vol 3)
4-ETHYL-o-XYLENE.....	187(Vol 3)	1-HEXYNE.....	155(Vol 2)
5-ETHYL-m-XYLENE.....	188(Vol 3)	2-HEXYNE.....	156(Vol 2)
FLUORANTHENE.....	309(Vol 3)	3-HEXYNE.....	157(Vol 2)
FLUORENE.....	272(Vol 3)	HYDRACRYLONITRILE.....	156(Vol 1)
FLUOROBENZENE.....	115(Vol 2)	HYDRAZOBENZENE.....	251(Vol 3)
FORMALDEHYDE.....	24(Vol 1)	HYDROGEN CYANIDE.....	18(Vol 1)
FORMAMIDE.....	31(Vol 1)	p-HYDROQUINONE.....	131(Vol 2)
FORMANILIDE.....	289(Vol 2)	p-HYDROXYBENZALDEHYDE.....	282(Vol 2)
FORMIC ACID.....	25(Vol 1)	HYDROXYCAPROIC ACID.....	211(Vol 2)
FUMARIC ACID.....	220(Vol 1)	2-HYDROXYETHYL ACRYLATE.....	33(Vol 2)
FURAN.....	217(Vol 1)	8-HYDROXYQUINOLINE.....	106(Vol 3)
FURFURAL.....	2(Vol 2)	INDANE.....	109(Vol 3)
FURFURYL ALCOHOL.....	9(Vol 2)	INDENE.....	107(Vol 3)
L-GLUTAMIC ACID.....	40(Vol 2)	INDOLE.....	7(Vol 3)
GLUTARIC ACID.....	36(Vol 2)	IODOBENZENE.....	116(Vol 2)
GLUTARIC ANHYDRIDE.....	10(Vol 2)	ISOBUTANE.....	291(Vol 1)
GLUTARONITRILE.....	8(Vol 2)	ISOBUTANOL.....	298(Vol 1)
GLYCEROL.....	197(Vol 1)	ISOBUTENE.....	264(Vol 1)
GLYCERYL TRIACETATE.....	130(Vol 3)	ISOBUTYL ACETATE.....	204(Vol 2)
GUAIACOL.....	300(Vol 2)	ISOBUTYL ACRYLATE.....	312(Vol 2)
HALOTHANE.....	58(Vol 1)	ISOBUTYL FORMATE.....	55(Vol 2)
n-HEPTADECANE.....	323(Vol 3)	ISOBUTYL ISOBUTYRATE.....	64(Vol 3)
1-HEPTADECANOL.....	324(Vol 3)	ISOBUTYL MERCAPTAN.....	308(Vol 1)
1-HEPTADECENE.....	322(Vol 3)	ISOBUTYLAMINE.....	314(Vol 1)
1-HEPTANAL.....	336(Vol 2)	ISOBUTYLBENZENE.....	189(Vol 3)
n-HEPTANE.....	359(Vol 2)	ISOBUTYRALDEHYDE.....	267(Vol 1)
n-HEPTANOIC ACID.....	350(Vol 2)	ISOBUTYRIC ACID.....	274(Vol 1)
1-HEPTANOL.....	363(Vol 2)	ISOBUTYRONITRILE.....	255(Vol 1)
2-HEPTANOL.....	364(Vol 2)	ISODECANOL.....	223(Vol 3)
2-HEPTANONE.....	335(Vol 2)	ISOPENTANE.....	70(Vol 2)
1-HEPTENE.....	324(Vol 2)	ISOPENTYL ACETATE.....	347(Vol 2)
cis-2-HEPTENE.....	325(Vol 2)	ISOPENTYL ISOVALERATE.....	214(Vol 3)

ISOPHORONE.....	129(Vol 3)
ISOPHTHALIC ACID.....	3(Vol 3)
ISOPHTHALOYL CHLORIDE.....	1(Vol 3)
ISOPRENE.....	16(Vol 2)
ISOPROPANOL.....	190(Vol 1)
ISOPROPYL ACETATE.....	56(Vol 2)
ISOPROPYL CHLORIDE.....	179(Vol 1)
ISOPROPYL IODIDE.....	181(Vol 1)
ISOPROPYL MERCAPTAN.....	199(Vol 1)
ISOPROPYLAMINE.....	201(Vol 1)
ISOPROPYLCYCLOHEXANE.....	132(Vol 3)
ISOQUINOLINE.....	104(Vol 3)
ISOVALERIC ACID.....	60(Vol 2)
ITACONIC ACID.....	12(Vol 2)
KETENE.....	79(Vol 1)
LACTIC ACID.....	174(Vol 1)
LACTONITRILE.....	157(Vol 1)
LEVULINIC ACID.....	34(Vol 2)
D-LIMONENE.....	197(Vol 3)
LINOLEIC ACID.....	335(Vol 3)
LYSINE.....	221(Vol 2)
MALEIC ACID.....	221(Vol 1)
MALEIC ANHYDRIDE.....	214(Vol 1)
MALIC ACID.....	252(Vol 1)
MALONONITRILE.....	134(Vol 1)
3-MERCAPTOPROPIONIC ACID.....	173(Vol 1)
MESITYL OXIDE.....	159(Vol 2)
MESITYLENE.....	122(Vol 3)
METHACROLEIN.....	241(Vol 1)
2-METHACRYLAMIDE.....	257(Vol 1)
METHACRYLIC ACID.....	246(Vol 1)
METHACRYLONITRILE.....	226(Vol 1)
METHANE.....	33(Vol 1)
METHANESULFONIC ACID.....	36(Vol 1)
METHANOL.....	35(Vol 1)
METHOXYACETIC ACID.....	175(Vol 1)
2-METHOXYETHANOL.....	193(Vol 1)
2-(2-METHOXYETHOXY)ETHANOL.....	88(Vol 2)
p-METHOXYPHENOL.....	301(Vol 2)
3-METHOXYPROPIONITRILE.....	258(Vol 1)
METHYL ACETATE.....	171(Vol 1)
METHYL ACETOACETATE.....	35(Vol 2)
METHYL ACRYLATE.....	247(Vol 1)
METHYL BENZOATE.....	11(Vol 3)
METHYL BROMIDE.....	26(Vol 1)
METHYL sec-BUTYL ETHER.....	81(Vol 2)
METHYL tert-BUTYL ETHER.....	82(Vol 2)
METHYL n-BUTYRATE.....	58(Vol 2)
METHYL CHLORIDE.....	27(Vol 1)
METHYL CHLOROACETATE.....	151(Vol 1)
METHYL CHLOROFORMATE.....	87(Vol 1)
METHYL CHLOROSILANE.....	38(Vol 1)
METHYL CYANOACETATE.....	229(Vol 1)
METHYL DICHLOROSILANE.....	34(Vol 1)
METHYL DIETHANOLAMINE.....	92(Vol 2)
METHYL DODECANOATE.....	279(Vol 3)
METHYL ETHYL ETHER.....	191(Vol 1)
METHYL ETHYL KETONE.....	269(Vol 1)
METHYL FLUORIDE.....	29(Vol 1)
METHYL FORMATE.....	105(Vol 1)
METHYL IODIDE.....	30(Vol 1)
METHYL ISOBUTYL ETHER.....	83(Vol 2)
METHYL ISOBUTYL KETONE.....	197(Vol 2)
METHYL ISOCYANATE.....	93(Vol 1)
METHYL ISOPROPENYL KETONE.....	27(Vol 2)
METHYL ISOPROPYL ETHER.....	297(Vol 1)
METHYL ISOPROPYL KETONE.....	49(Vol 2)
METHYL MERCAPTAN.....	37(Vol 1)
METHYL METHACRYLATE.....	31(Vol 2)
METHYL OLEATE.....	346(Vol 3)
METHYL tert-PENTYL ETHER.....	230(Vol 2)
METHYL PROPIONATE.....	278(Vol 1)
METHYL SALICYLATE.....	14(Vol 3)
METHYL SILANE.....	40(Vol 1)
3-METHYL SULFOLANE.....	63(Vol 2)
METHYL TRICHLOROSILANE.....	28(Vol 1)
METHYL VINYL ETHER.....	166(Vol 1)
N-METHYLACETAMIDE.....	186(Vol 1)

METHYLACETYLENE.....	138(Vol 1)
METHYLAL.....	194(Vol 1)
METHYLAMINE.....	39(Vol 1)
N-METHYLANILINE.....	304(Vol 2)
2-METHYLBENZOFURAN.....	108(Vol 3)
3-METHYL-1,2-BUTADIENE.....	17(Vol 2)
2-METHYL-1-BUTANOL.....	74(Vol 2)
2-METHYL-2-BUTANOL.....	75(Vol 2)
3-METHYL-1-BUTANOL.....	76(Vol 2)
3-METHYL-2-BUTANOL.....	77(Vol 2)
2-METHYL-2-BUTENE.....	43(Vol 2)
2-METHYL-1-BUTENE.....	42(Vol 2)
3-METHYL-1-BUTENE.....	44(Vol 2)
2-METHYL-1-BUTENE-3-YNE.....	5(Vol 2)
3-METHYL-1-BUTYNE.....	24(Vol 2)
2-METHYLBUTYRIC ACID.....	59(Vol 2)
METHYLCYCLOHEXANE.....	329(Vol 2)
1-METHYLCYCLOHEXANOL.....	337(Vol 2)
cis-2-METHYLCYCLOHEXANOL.....	338(Vol 2)
cis-3-METHYLCYCLOHEXANOL.....	340(Vol 2)
cis-4-METHYLCYCLOHEXANOL.....	342(Vol 2)
trans-2-METHYLCYCLOHEXANOL.....	339(Vol 2)
trans-3-METHYLCYCLOHEXANOL.....	341(Vol 2)
trans-4-METHYLCYCLOHEXANOL.....	343(Vol 2)
N-METHYLCYCLOHEXYLAMINE.....	353(Vol 2)
METHYLCYCLOPENTADIENE.....	139(Vol 2)
METHYLCYCLOPENTANE.....	182(Vol 2)
METHYLETHANOLAMINE.....	205(Vol 1)
1-METHYL-1-ETHYLCYCLOPENTANE.....	51(Vol 3)
3-METHYL-3-ETHYLPENTANE.....	74(Vol 3)
N-METHYLFORMAMIDE.....	113(Vol 1)
METHYLGLUTARONITRILE.....	141(Vol 2)
2-METHYLHEPTANE.....	75(Vol 3)
3-METHYLHEPTANE.....	76(Vol 3)
4-METHYLHEPTANE.....	77(Vol 3)
2-METHYLHEXANE.....	360(Vol 2)
3-METHYLHEXANE.....	361(Vol 2)
5-METHYL-1-HEXANOL.....	365(Vol 2)
5-METHYL-2-HEXANONE.....	344(Vol 2)
2-METHYL-1-HEXENE.....	330(Vol 2)
3-METHYL-1-HEXENE.....	331(Vol 2)
4-METHYL-1-HEXENE.....	332(Vol 2)
1-METHYLINDENE.....	166(Vol 3)
2-METHYLINDENE.....	167(Vol 3)
1-METHYLNAPHTHALENE.....	227(Vol 3)
2-METHYLNAPHTHALENE.....	228(Vol 3)
2-METHYLNONANE.....	217(Vol 3)
3-METHYLNONANE.....	218(Vol 3)
4-METHYLNONANE.....	219(Vol 3)
5-METHYLNONANE.....	220(Vol 3)
2-METHYLOCTANE.....	146(Vol 3)
3-METHYLOCTANE.....	147(Vol 3)
4-METHYLOCTANE.....	148(Vol 3)
2-METHYLPENTANE.....	219(Vol 2)
3-METHYLPENTANE.....	220(Vol 2)
2-METHYL-1-PENTANOL.....	225(Vol 2)
4-METHYL-2-PENTANOL.....	226(Vol 2)
2-METHYL-1-PENTENE.....	183(Vol 2)
2-METHYL-2-PENTENE.....	184(Vol 2)
3-METHYL-1-PENTENE.....	185(Vol 2)
4-METHYL-1-PENTENE.....	187(Vol 2)
3-METHYL-cis-2-PENTENE.....	186(Vol 2)
4-METHYL-cis-2-PENTENE.....	188(Vol 2)
4-METHYL-trans-2-PENTENE.....	189(Vol 2)
2-METHYLPYRIDINE.....	135(Vol 2)
3-METHYLPYRIDINE.....	136(Vol 2)
4-METHYLPYRIDINE.....	137(Vol 2)
N-METHYLPYRROLE.....	13(Vol 2)
N-METHYLPYRROLIDINE.....	67(Vol 2)
N-METHYL-2-PYRROLIDONE.....	39(Vol 2)
alpha-METHYLSTYRENE.....	110(Vol 3)
m-METHYLSTYRENE.....	111(Vol 3)
o-METHYLSTYRENE.....	112(Vol 3)
p-METHYLSTYRENE.....	113(Vol 3)
MONOCHLOROENZENE.....	110(Vol 2)
MONOETHANOLAMINE.....	127(Vol 1)
MORPHOLINE.....	289(Vol 1)
NAPHTHALENE.....	163(Vol 3)

NEOPENTANE.....	71(Vol 2)	trans-2-PENTENE.....	47(Vol 2)
NEOPENTYL GLYCOL.....	86(Vol 2)	1-PENTENE-3-YNE.....	6(Vol 2)
m-NITROANILINE.....	125(Vol 2)	1-PENTENE-4-YNE.....	7(Vol 2)
o-NITROANILINE.....	126(Vol 2)	n-PENTYL ACETATE.....	348(Vol 2)
p-NITROANILINE.....	127(Vol 2)	n-PENTYL FORMATE.....	198(Vol 2)
o-NITROANISOLE.....	293(Vol 2)	n-PENTYL MERCAPTAN.....	90(Vol 2)
NITROBENZENE.....	117(Vol 2)	n-PENTYLAMINE.....	91(Vol 2)
3-NITROBENZOTRIFLUORIDE.....	265(Vol 2)	n-PENTYLBENZENE.....	230(Vol 3)
NITROETHANE.....	114(Vol 1)	1-PENTYNE.....	23(Vol 2)
NITROGLYCERINE.....	158(Vol 1)	alpha-PHELLANDRENE.....	198(Vol 3)
NITROMETHANE.....	32(Vol 1)	beta-PHELLANDRENE.....	199(Vol 3)
1-NITROPROPANE.....	187(Vol 1)	PHENANTHRENE.....	285(Vol 3)
2-NITROPROPANE.....	188(Vol 1)	p-PHENETIDINE.....	34(Vol 3)
m-NITROTOLUENE.....	290(Vol 2)	PHENETOLE.....	23(Vol 3)
o-NITROTOLUENE.....	291(Vol 2)	PHENOL.....	128(Vol 2)
p-NITROTOLUENE.....	292(Vol 2)	PHENYL ISOCYANATE.....	271(Vol 2)
n-NONADECANE.....	349(Vol 3)	PHENYL MERCAPTAN.....	133(Vol 2)
NONADECANOIC ACID.....	348(Vol 3)	m-PHENYLENEDIAMINE.....	142(Vol 2)
1-NONADECENE.....	347(Vol 3)	o-PHENYLENEDIAMINE.....	143(Vol 2)
1-NONANAL.....	136(Vol 3)	p-PHENYLENEDIAMINE.....	144(Vol 2)
n-NONANE.....	149(Vol 3)	2-PHENYLETHANOL.....	24(Vol 3)
n-NONANOIC ACID.....	138(Vol 3)	PHENYLHYDRAZINE.....	145(Vol 2)
1-NONANOL.....	155(Vol 3)	1-PHENYLNAPHTHALENE.....	311(Vol 3)
2-NONANOL.....	156(Vol 3)	2-PHENYL-2-PROPANOL.....	127(Vol 3)
1-NONENE.....	133(Vol 3)	PHOSGENE.....	8(Vol 1)
n-NONYL MERCAPTAN.....	157(Vol 3)	PTHALIC ACID.....	4(Vol 3)
n-NONYLAMINE.....	158(Vol 3)	PTHALIC ANHYDRIDE.....	2(Vol 3)
n-NONYLBENZENE.....	303(Vol 3)	alpha-PINENE.....	200(Vol 3)
1-n-NONYLNAPHTHALENE.....	344(Vol 3)	beta-PINENE.....	201(Vol 3)
NONYLPHENOL.....	305(Vol 3)	PIPERAZINE.....	292(Vol 1)
2-NORBORNENE.....	308(Vol 2)	PIPERIDINE.....	68(Vol 2)
n-OCTADECANE.....	341(Vol 3)	PROPADIENE.....	139(Vol 1)
1-OCTADECANOL.....	343(Vol 3)	PROPANE.....	189(Vol 1)
1-OCTADECENE.....	339(Vol 3)	1,2-PROPANEDIAMINE.....	207(Vol 1)
OCTAFLUORO-2-BUTENE.....	211(Vol 1)	n-PROPANOL.....	192(Vol 1)
OCTAFLUOROCYCLOBUTANE.....	212(Vol 1)	PROPARGYL ALCOHOL.....	142(Vol 1)
OCTAFLUOROPROPANE.....	133(Vol 1)	PROPARGYL CHLORIDE.....	135(Vol 1)
OCTAMETHYLCYCLOTETRASILOXANE.....	101(Vol 3)	beta-PROPIOLACTONE.....	144(Vol 1)
1-OCTANAL.....	60(Vol 3)	n-PROPIONALDEHYDE.....	167(Vol 1)
n-OCTANE.....	78(Vol 3)	PROPIONIC ACID.....	172(Vol 1)
n-OCTANOIC ACID.....	65(Vol 3)	PROPIONIC ANHYDRIDE.....	164(Vol 2)
1-OCTANOL.....	87(Vol 3)	PROPIONITRILE.....	154(Vol 1)
2-OCTANOL.....	88(Vol 3)	n-PROPYL ACETATE.....	57(Vol 2)
2-OCTANONE.....	61(Vol 3)	n-PROPYL ACRYLATE.....	162(Vol 2)
1-OCTENE.....	52(Vol 3)	n-PROPYL n-BUTYRATE.....	349(Vol 2)
trans-2-OCTENE.....	53(Vol 3)	n-PROPYL CHLORIDE.....	180(Vol 1)
trans-3-OCTENE.....	54(Vol 3)	n-PROPYL FORMATE.....	279(Vol 1)
trans-4-OCTENE.....	55(Vol 3)	n-PROPYL IODIDE.....	182(Vol 1)
n-OCTYL FORMATE.....	139(Vol 3)	n-PROPYL METHACRYLATE.....	313(Vol 2)
n-OCTYL MERCAPTAN.....	95(Vol 3)	n-PROPYL PROPIONATE.....	205(Vol 2)
t-OCTYL MERCAPTAN.....	96(Vol 3)	n-PROPYLAMINE.....	200(Vol 1)
n-OCTYLAMINE.....	99(Vol 3)	n-PROPYLBENZENE.....	123(Vol 3)
n-OCTYLBENZENE.....	293(Vol 3)	n-PROPYLCYCLOHEXANE.....	134(Vol 3)
p-tert-OCTYLPHENOL.....	294(Vol 3)	n-PROPYLCYCLOPENTANE.....	56(Vol 3)
OLEIC ACID.....	336(Vol 3)	PROPYLENE.....	160(Vol 1)
OXALIC ACID.....	80(Vol 1)	1,2-PROPYLENE GLYCOL.....	195(Vol 1)
OXAZOLE.....	137(Vol 1)	1,3-PROPYLENE GLYCOL.....	196(Vol 1)
PARALDEHYDE.....	212(Vol 2)	1,3-PROPYLENE OXIDE.....	169(Vol 1)
PENTACHLOROETHANE.....	63(Vol 1)	1,2-PROPYLENE OXIDE.....	168(Vol 1)
n-PENTADECANE.....	308(Vol 3)	PROPYLENEIMINE.....	184(Vol 1)
PENTADECANOIC ACID.....	307(Vol 3)	n-PROPYLMERCAPTAN.....	198(Vol 1)
1-PENTADECENE.....	306(Vol 3)	PYRENE.....	310(Vol 3)
1,2-PENTADIENE.....	18(Vol 2)	PYRIDINE.....	3(Vol 2)
1,4-PENTADIENE.....	21(Vol 2)	PYROMELLITIC ACID.....	160(Vol 3)
2,3-PENTADIENE.....	22(Vol 2)	PYRROLE.....	227(Vol 1)
cis-1,3-PENTADIENE.....	19(Vol 2)	PYRROLIDINE.....	287(Vol 1)
trans-1,3-PENTADIENE.....	20(Vol 2)	2-PYRROLIDONE.....	259(Vol 1)
PENTAERYTHRITOL.....	89(Vol 2)	PYRUVIC ACID.....	147(Vol 1)
PENTAERYTHRITOL TETRANITRATE.....	25(Vol 2)	QUINALDINE.....	164(Vol 3)
PENTAFLUOROETHANE.....	65(Vol 1)	QUINOLINE.....	105(Vol 3)
n-PENTANE.....	72(Vol 2)	SALICYLALDEHYDE.....	283(Vol 2)
1,5-PENTANEDIOL.....	87(Vol 2)	SALICYLIC ACID.....	284(Vol 2)
1-PENTANOL.....	78(Vol 2)	SEBACIC ACID.....	208(Vol 3)
2-PENTANOL.....	79(Vol 2)	SORBITOL.....	241(Vol 2)
3-PENTANOL.....	80(Vol 2)	STEARIC ACID.....	340(Vol 3)
2-PENTANONE.....	50(Vol 2)	cis-STILBENE.....	286(Vol 3)
1-PENTENE.....	45(Vol 2)	trans-STILBENE.....	287(Vol 3)
cis-2-PENTENE.....	46(Vol 2)	STYRENE.....	8(Vol 3)

SUCCINIC ACID.....250(Vol 1)
 SUCCINIC ANHYDRIDE.....219(Vol 1)
 SUCCINONITRILE.....216(Vol 1)
 SULFOLANE.....280(Vol 1)
 TARTARIC ACID.....253(Vol 1)
 TEREPHTHALIC ACID.....5(Vol 3)
 m-TERPHENYL.....326(Vol 3)
 o-TERPHENYL.....327(Vol 3)
 p-TERPHENYL.....328(Vol 3)
 alpha-TERPINENE.....202(Vol 3)
 gamma-TERPINENE.....203(Vol 3)
 TERPINOLENE.....204(Vol 3)
 1,1,2,2-TETRABROMOETHANE.....67(Vol 1)
 1,1,2,2-TETRACHLORODIFLUOROETHANE...53(Vol 1)
 1,1,1,2-TETRACHLOROETHANE.....75(Vol 1)
 1,1,2,2-TETRACHLOROETHANE.....76(Vol 1)
 TETRACHLOROETHYLENE.....52(Vol 1)
 TETRACHLOROTHIOPHENE...209(Vol 1)
 n-TETRADECANE.....297(Vol 3)
 n-TETRADECANOIC ACID.....296(Vol 3)
 1-TETRADECANOL.....298(Vol 3)
 1-TETRADECENE.....295(Vol 3)
 TETRADECYLAMINE.....299(Vol 3)
 TETRAETHYLENE GLYCOL...94(Vol 3)
 TETRAETHYLENE GLYCOL DIMETHYL ETHER.224(Vol 3)
 TETRAETHYLENEPENTAMINE.....100(Vol 3)
 1,1,1,2-TETRAFLUOROETHANE.....78(Vol 1)
 TETRAFLUOROETHYLENE.....56(Vol 1)
 TETRAHYDROFURAN.....271(Vol 1)
 TETRAHYDROFURFURYL ALCOHOL.....62(Vol 2)
 1,2,3,4-TETRAHYDRONAPHTHALENE.....171(Vol 3)
 TETRAHYDROTHIOPHENE.....281(Vol 1)
 1,2,3,5-TETRAMETHYLBENZENE.....190(Vol 3)
 1,2,4,5-TETRAMETHYLBENZENE.....191(Vol 3)
 2,2,3,3-TETRAMETHYLPENTANE.....150(Vol 3)
 2,2,3,4-TETRAMETHYLPENTANE.....151(Vol 3)
 2,2,4,4-TETRAMETHYLPENTANE.....152(Vol 3)
 TETRAMETHYLSILANE.....322(Vol 1)
 TETRANITROMETHANE.....41(Vol 1)
 TETRAPHENYLETHYLENE.....362(Vol 3)
 THIOPHENE.....222(Vol 1)
 p-TOLUALDEHYDE.....10(Vol 3)
 TOLUENE.....294(Vol 2)
 TOLUENE DIISOCYANATE.....103(Vol 3)
 TOLUENEDIAMINE.....309(Vol 2)
 o-TOLUIC ACID.....12(Vol 3)
 p-TOLUIC ACID.....13(Vol 3)
 m-TOLUIDINE.....305(Vol 2)
 o-TOLUIDINE.....306(Vol 2)
 p-TOLUIDINE.....307(Vol 2)
 TRIBROMOMETHANE.....13(Vol 1)
 TRI-n-BUTYL BORATE.....269(Vol 3)
 TRI-n-BUTYLAMINE.....271(Vol 3)
 TRICHLOROACETALDEHYDE.....62(Vol 1)
 TRICHLOROACETYL CHLORIDE.....54(Vol 1)
 1,2,4-TRICHLOROBENZENE.....97(Vol 2)
 1,1,1-TRICHLOROETHANE.....88(Vol 1)
 1,1,2-TRICHLOROETHANE.....89(Vol 1)
 TRICHLOROETHYLENE.....60(Vol 1)
 1,1,1-TRICHLOROFUOROETHANE.....74(Vol 1)
 TRICHLOROFUOROMETHANE.....9(Vol 1)
 1,2,3-TRICHLOROPROPANE.....153(Vol 1)
 1,1,2-TRICHLOROTRIFLUOROETHANE.....51(Vol 1)
 TRI-o-CRESYL PHOSPHATE.....357(Vol 3)
 1-TRIDECANAL.....277(Vol 3)
 n-TRIDECANE.....280(Vol 3)
 1-TRIDECANOL.....281(Vol 3)
 1-TRIDECENE.....276(Vol 3)
 n-TRIDECYLBENZENE.....345(Vol 3)
 TRIETHANOLAMINE.....251(Vol 2)
 TRIETHYL ALUMINUM.....243(Vol 2)
 TRIETHYL PHOSPHATE.....253(Vol 2)
 TRIETHYLAMINE.....248(Vol 2)
 TRIETHYLENE GLYCOL.....240(Vol 2)
 TRIETHYLENE GLYCOL DIMETHYL ETHER...93(Vol 3)
 TRIETHYLENE TETRAMINE.....256(Vol 2)
 TRIETHYLENEDIAMINE.....190(Vol 2)
 TRIFLUOROACETIC ACID.....64(Vol 1)

1,1,1-TRIFLUOROETHANE.....91(Vol 1)
 TRIFLUOROMETHANE.....17(Vol 1)
 TRIMELLITIC ANHYDRIDE.....102(Vol 3)
 TRIMETHYL PHOSPHATE.....206(Vol 1)
 TRIMETHYL SILANE.....208(Vol 1)
 TRIMETHYLAMINE.....202(Vol 1)
 1,2,3-TRIMETHYLBENZENE.....124(Vol 3)
 1,2,4-TRIMETHYLBENZENE.....125(Vol 3)
 2,2,3-TRIMETHYLBUTANE.....362(Vol 2)
 2,3,3-TRIMETHYL-1-BUTENE.....333(Vol 2)
 2,2,5-TRIMETHYLHEXANE.....153(Vol 3)
 1,2,3-TRIMETHYLINDENE.....252(Vol 3)
 TRIMETHYLOLPROPANE.....239(Vol 2)
 2,2,3-TRIMETHYLPENTANE.....79(Vol 3)
 2,2,4-TRIMETHYLPENTANE.....80(Vol 3)
 2,3,3-TRIMETHYLPENTANE.....81(Vol 3)
 2,3,4-TRIMETHYLPENTANE.....82(Vol 3)
 2,4,4-TRIMETHYL-1-PENTENE.....57(Vol 3)
 2,4,4-TRIMETHYL-2-PENTENE.....58(Vol 3)
 2,4,6-TRIMETHYLPYRIDINE.....33(Vol 3)
 1,3,5-TRINITROBENZENE.....98(Vol 2)
 2,4,6-TRINITROTOLUENE.....272(Vol 2)
 TRIPHENYL PHOSPHATE.....330(Vol 3)
 TRIPHENYLETHYLENE.....350(Vol 3)
 TRIPHENYLPHOSPHINE.....329(Vol 3)
 TRIOXANE.....176(Vol 1)
 TRIPROPYLAMINE.....159(Vol 3)
 1-UNDECANAL.....234(Vol 3)
 n-UNDECANE.....235(Vol 3)
 1-UNDECANOL.....236(Vol 3)
 1-UNDECENE.....233(Vol 3)
 UNDECYL MERCAPTAN.....237(Vol 3)
 n-UNDECYLBENZENE.....321(Vol 3)
 VALERALDEHYDE.....52(Vol 2)
 VALERIC ACID.....61(Vol 2)
 VALERONITRILE.....37(Vol 2)
 VANILLIN.....15(Vol 3)
 VINYL ACETATE.....248(Vol 1)
 VINYL BROMIDE.....81(Vol 1)
 VINYL CHLORIDE.....82(Vol 1)
 VINYL FLUORIDE.....90(Vol 1)
 VINYL FORMATE.....145(Vol 1)
 VINYL PROPIONATE.....32(Vol 2)
 VINYLACETONITRILE.....228(Vol 1)
 VINYLACETYLENE.....215(Vol 1)
 VINYL CYCLOHEXENE.....36(Vol 3)
 m-XYLENE.....18(Vol 3)
 o-XYLENE.....19(Vol 3)
 p-XYLENE.....20(Vol 3)
 2,3-XYLENOL.....25(Vol 3)
 2,4-XYLENOL.....26(Vol 3)
 2,5-XYLENOL.....27(Vol 3)
 2,6-XYLENOL.....28(Vol 3)
 3,4-XYLENOL.....29(Vol 3)
 3,5-XYLENOL.....30(Vol 3)

Appendix H

Computer Program for Thermodynamic Properties

A computer program for calculation of thermodynamic properties using the Peng-Robinson equation of state is available for a nominal fee (Carl L. Yaws, Box 10053, Lamar University, Beaumont, TX 77710, phone/FAX 409-880-8787). The computer program is executable and complete with data files. The program calculates thermodynamic properties at pressures and temperatures that are input by the user. Representative results are shown below:

COMPOUND: 440 C5H12 n-PENTANE

reference state: datum of ideal gas @ 77 F (25 C)

P psia	T F	Z	V ft ³ /lb	H BTU/lb	S BTU/lb F
-----	-----	-----	-----	-----	-----
500.0	-100.00	0.208	0.022	-242.63	-0.478
500.0	0.00	0.171	0.023	-196.52	-0.365
500.0	100.00	0.152	0.025	-144.08	-0.262
500.0	200.00	0.144	0.028	-84.27	-0.164
500.0	300.00	0.151	0.034	-14.40	-0.065
500.0	400.00	0.476	0.122	113.90	0.091
500.0	500.00	0.724	0.207	193.40	0.179
500.0	1000.00	0.963	0.418	580.50	0.501
3000.0	-100.00	1.232	0.022	-233.98	-0.482
3000.0	0.00	1.008	0.023	-188.53	-0.371
3000.0	100.00	0.875	0.024	-137.40	-0.270
3000.0	200.00	0.797	0.026	-80.30	-0.177
3000.0	300.00	0.758	0.029	-17.09	-0.087
3000.0	400.00	0.751	0.032	52.18	-0.002
3000.0	500.00	0.772	0.037	127.06	0.080
3000.0	1000.00	1.006	0.073	549.91	0.433
10000.0	-100.00	4.024	0.022	-209.14	-0.491
10000.0	0.00	3.244	0.022	-164.63	-0.382
10000.0	100.00	2.757	0.023	-114.95	-0.285
10000.0	200.00	2.431	0.024	-60.03	-0.194
10000.0	300.00	2.204	0.025	0.06	-0.110
10000.0	400.00	2.041	0.026	65.15	-0.029
10000.0	500.00	1.922	0.027	134.97	0.047
10000.0	1000.00	1.649	0.036	544.22	0.388